Atomic Structure of the Catalytic Domain for Use in Designing and Identifying Inhibitors of ZAP-70 Kinase

Field of the Invention

The present invention relates to ZAP-70 protein tyrosine kinase, in particular, the three-dimensional structure of the catalytic domain of ZAP-70 protein tyrosine kinase. The invention also relates to the crystalline forms of liganded or unliganded human ZAP-70 catalytic domain. Further, the invention describes methods of making of a crystal comprising ZAP-70 and purification of the catalytic domain of ZAP-70 for use in crystallization. The invention also relates to the use of the three-dimensional structure of the catalytic domain of ZAP-70 kinase for identifying and designing ligands or low molecular weight compounds which inhibit the biological function of ZAP-70.

Background of the Invention

The protein tyrosine kinase ZAP-70 (zeta chain-associated protein of 70 kDa) plays a pivotal role in T cell activation. T cells are involved in transplant rejection, autoimmune diseases and the initiation of inflammatory responses. Activation of T cells requires engagement of the antigen-specific T cell receptor (TCR), resulting in early membrane proximal events which lead to the activation of a number of signal transduction pathways.

One of the early events of T cell activation is the phosphorylation of the TCR zeta chain and the specific association and activation of the Syk family protein tyrosine kinase ZAP-70 with the TCR via its two SH2 domains. Zeta chain-binding together with trans-phosphorylation by the src family kinase Lck leads to the activation of ZAP-70. ZAP-70 phosphorylates its specific substrate LAT (linker for activation of T cells), an adaptor molecule, which then recruits a number of downstream effector molecules. This eventually leads to the activation of early T cell genes, production of cytokines and cellular proliferation. There is ample evidence that interference with ZAP-70/LAT-mediated signaling leads to functional T cell inactivation.

Defects in ZAP-70 are the cause of selective T cell defect (STD), an autosomal recessive form of severe combined immunodeficiency characterized by a selective absence of CD-8-type T cells.

The crystal structure of the tandem SH2 domains of human ZAP-70 in complex with a peptide derived from the TCR zeta chain has been previously described by Hatada et al.

(1995). This three-dimensional crystal structure of the SH2 domain has also been the subject of US patent 6,251,620. The disclosure of this SH2 domain has lead to efforts directed at blocking the ZAP-70 SH2 domain/zeta chain interaction. However, to date no orally active inhibitor of ZAP-70 has been described.

The present invention focuses on the three dimensional structure of the catalytic domain of ZAP-70 for inhibition of ZAP-70 since catalytic activity at the ATP-binding site can be directly inhibited. Before the disclosure of the present invention, there was no three-dimensional crystal structure of the catalytic domain of ZAP-70. With the three-dimensional structure of the catalytic domain of the human ZAP-70, identifying and designing inhibitors of ZAP-70 based on the three-dimensional structure of the catalytic domain is now possible.

Summary of the Invention

It is an object of the present invention to provide the three-dimensional structure of ZAP-70 kinase catalytic domain thereby enabling identification and design of ligands or low molecular weight molecules that specifically inhibit ZAP-70 kinase.

The present invention relates to:

(i) a crystal of the ZAP-70 kinase comprising the catalytic domain of ZAP-70 kinase with or without a ligand or low molecular weight compound

(ii) a method of making a crystal of ZAP-70 kinase comprising the ZAP-70 kinase catalytic domain

(iii) methods of using said ZAP-70 kinase crystal comprising the catalytic domain and its structural coordinates.

The three-dimensional structural information revealed from the crystal of the the catalytic domain of ZAP-70 kinase can be used for structure-based drug discovery for screening, identifying and designing inhibitors of ZAP-70 kinase.

Detailed Description of the Invention

The full-length sequence of human ZAP-70 kinase is known and set forth in Genbank Accession number L05148 and SwissProt Accession number P43403, which are incorporated herein by reference.

The present invention provides ZAP-70 kinase catalytic domain in crystallized form. In particular, it provides a crystal comprising the catalytic domain of ZAP-70 kinase and a ligand bound to ZAP-70 as a complex.

In one embodiment of the present invention, a crystal of the catalytic domain of ZAP-70 kinase comprising a unit cell dimension of a = 35.77 ± 5 Ångstroms   b =   57.56 ± 5 Ångstroms c = 80.20 ± 5 Ångstroms , α= 68.97 ± 5 degrees β = 89.83 ± 5 degrees γ = 89.95 ± 5 degrees is provided. Depending on the particular conditions for crystallization, the parameters characterising the unit cell may vary with a limited range, for example, a,b,c each vary by up to 5 Ångstroms and α, β, γ each vary by up to 5 degrees. The space group of the present invention is P1 primitive triclinic.

The term "unit cell" according to the invention refers to the basic shape block. The entire volume of a crystal may be constructed by regular assembly of such blocks. Each unit cell comprises a complete representation of the unit of pattern, the repetition of which builds up the crystal.

The term "space group" according to the invention refers to the arrangement of symmetry elements of a crystal.

In another embodiment of the invention, a crystal of ZAP-70 kinase comprising the catalytic domain of ZAP-70 kinase in complex with a ligand is provided wherein said crystal has a three-dimensional structure characterized by the atomic structure coordinates of Table 1.

In a further embodiment of the invention, said catalytic domain of ZAP-70 kinase comprises the sequence of SEQ ID. No. 2, fragment or homologue thereof.

In yet another embodiment of the invention, said catalytic domain of ZAP-70 kinase comprises at least the ATP-binding site.

Further provided by this invention is a crystal comprising the catalytic domain of ZAP-70 bound to at least one ligand or low molecular weight compound.

The term "ligand" according to the invention, refers to a molecule or group of molecules that bind to one or more specific sites of ZAP-70, preferably to the catalytic domain of ZAP-70 and most preferably to the ATP binding-site of said catalytic domain. Ligands according to the invention are preferably low molecular weight molecules.

The term "low molecular weight compound" according to the invention refers to preferably organic compounds generally having a molecular weight less than about 1000, more preferably less than about 500. Most preferably, said low molecular weight compounds or ligands inhibit ZAP-70 biological activity.

In context of a ZAP-70 inhibitor, the terms "peptide" or "peptide derivative" are intended to embrace a "peptidomimetic" or "peptide analogue" which complement the three-dimensional structure of the binding site of ZAP-70 kinase or can be designed with improved physical or chemical properties to bind with the three-dimensional binding site of the ZAP-70 kinase catalytic domain as provided in the present invention.

The term "mutant" refers to differences in the wild-type sequence of ZAP-70 kinase set forth in Genbank Accession number L05148 or SwissProt Accession number P43403 by deletion, insertion or preferably replacement of one or more selected amino acids.

According to the present invention, the term "mutant" also refers to a polypeptide, whose amino acid sequence differs from the wild-type sequence given in SEQ ID No.2 by deletion, insertion or preferably replacement of one or more selected amino acids. For example, a ZAP-70 mutant of the catalytic domain of the present invention is preferably at least 50% homologous to SEQ ID No. 2, more preferably at least 80% homologous to SEQ ID No. 2 most preferably at least 90% homologous to SEQ ID No. 2.

A "fragment" of ZAP-70 catalytic domain according to the invention comprises more than 50% of the full-length sequence of the ZAP-70 catalytic domain according to SEQ ID No. 2, more preferably at least 80% of the full-length sequence of the ZAP-70 catalytic domain according to SEQ ID No. 2, most preferably at least 90% of the full-length sequence of the ZAP-70 catalytic domain according to SEQ ID No. 2.

In one embodiment of the invention, a ZAP-70 mutant of the catalytic domain may be crystallizable with or without at least one ligand.

In another embodiment of the invention, a ZAP-70 fragment of the catalytic domain may be crystallizable with or without at least one ligand.

In yet another embodiment of the invention, a method is provided wherein the catalytic domain of ZAP-70, a fragment or homologue thereof is bound to at least one ligand at any step prior to crystallization.

According to the present invention, ZAP-70 crystals are stable for at least one month, if kept under suitable conditions. Hepes pH 7.2 is identified as being suitable for the concentration of ZAP-70 without precipitation. Initially during purification, high concentrations of glycerol (30-50%v/v) are preferred, below which rapid precipitation occurs at protein concentrations in excess of 5 - 10mg/ml. During the final concentration steps 1%v/v ethylene glycol can substitute for glycerol allowing concentrations in excess of 30mg/ml to be reached. An additional cation-exchange step is also recommended to remove incorrectly folded or unstable ZAP-70 which interferes with the concentration and crystallisation process.

The purified protein ZAP-70 catalytic domain of SEQ. ID No.2, homologue or fragment thereof is advantageously obtainable according to method of the present invention by initial expression of the full-length ZAP-70 SEQ ID No.1 flanked by protease recognition sequences. This facilitates efficient proteolytic release of the desired domain. This method is preferable to standard methods known in the art whereby the desired domain typically is isolated from the full-length protein and then expressed.

Purification of an N-terminally tagged full-length ZAP-70 using a nickel-chelating affinity column yields protein of limited purity which cannot be easily purified by additional "standard" chromatographic procedures such as ion-exchange or size-exclusion chromatography. According to the present invention, affinity chromatography using γ-aminophenyl-ATP sepharose is the preferred means of purification leading to a high purity the ZAP-70 protein. Identification of the desired ZAP-70 catalytic domain is preferably by immunochemical method, for example, Western-blotting.

In one embodiment of the invention, a method for making a crystal of a ZAP-70 kinase is provided comprising the following steps:

(i) purification of the full-length ZAP-70 kinase (SEQ ID No.1)

(ii) proteolytic domain definition

(iii) expression of the full-length ZAP-70 kinase of SEQ ID No.1 flanked by protease recognition sequences to facilitate proteolytic release of the desired domain of ZAP-70

(iv) expression of the full-length ZAP-kinase from step (iii) in a suitable host cell

(v) controlled proteolysis of the desired domain at protease recognition sites

(vi) rapid purification of the desired ZAP-70 domain.

In a preferred embodiment of the invention, said method for making a crystal comprises the desired domain of ZAP-70 kinase domain comprising the catalytic domain of ZAP-70 kinase of SEQ ID No.2, a fragment or homologue thereof.

According to the invention, ZAP-70 may be prepared by isolation from natural sources, e.g. cultured human cells or preferably by recombinant heterologous expression. Expression of recombinant ZAP-70 is achievable in eukaryotic or prokaryotic systems. For example, recombinant human ZAP-70 may be expressed in insect cells, such as Sf9 cells, using a suitable recombinant baculovirus system or in bacteria.

The kinase may be expressed as a fusion protein, e.g. a glutathione-S-transferase (GST) or histidine-tagged fusion protein. If desired, the fusion partner is removed before crystallization. The heterologously produced ZAP-70 to be used for crystallization is biologically active. Such ability may be determined by morphological, biochemical or viability analysis well-known in the art.

Methods for the preparation of ZAP-70 mutants are commonly known in the art. For example, ZAP-70 mutants may be prepared by expression of ZAP-70 DNA previously modified in its coding region by oligo-nucleotide directed mutagenesis.

In the present invention, purified ZAP-70 is preferably at least 90 % homogeneous. Protein homogeneity is determinable according to analytical methods well-known in the art, e.g. sequence analysis, electrophoresis, spectroscopic or chromatographic techniques. The

purified protein is enzymatically active. Appropriate assays for determining ZAP-70 kinase activity towards a suitable substrate, e.g. a natural substrate or a synthetic substrate which is known in the art.

In one embodiment of the invention, prior to crystallization ZAP-70 may be reacted with a low molecular weight compound or ligand which is capable of suitably binding to the ZAP-70 catalytic domain site. Preferred is a compound inhibiting ZAP-70 activity. Kinase inhibition is determinable employing assays known in the art. Suitable inhibitors include ATP-competitive kinase inhibitors which act on the catalytic domain to inhibit ZAP-70 activity.

Various methods of cystallization can be used in the claimed invention including vapor diffusion, dialysis or batch crystallization. In vapor diffusion crystallization, a small volume (i.e., a few microliters) of protein solution is mixed with a solution containing a precipitant. This mixed volume is suspended over a well containing a small amount, i.e. about 1 ml, of precipitant. Vapor diffusion from the drop to the well will result in crystal formation in the drop.

The dialysis method of crystallization utilizes a semipermeable size-exclusion membrane that retains the protein but allows small molecules (i.e. buffers and precipitants) to diffuse in and out. In dialysis, rather than concentrating the protein and the precipitant by evaporation, the precipitant is allowed to slowly diffuse through the membrane and reduce the solubility of the protein while keeping the protein concentration fixed.

The batch method generally involves the slow addition of a precipitant to an aqueous solution of protein until the solution just becomes turbid, at this point the container can be sealed and left undisturbed for a period of time until crystallization occurs. In the batch technique the precipitant and the target molecule solution are simply mixed. Supersaturation is achieved directly rather than by diffusion. Often the batch technique is performed under oil. The oil prevents evaporation and extremely small drops can be used. For this, the term "microbatch" is used. A modification of this technique is not to use paraffin oil (which prevents evaporation completely) but rather use silicone oil or a mixture of silicone and paraffin oils so that a slow evaporation is possible.

The claimed invention can encompass any and all methods of crystallization. One skilled in the art can choose any of such methods and vary the parameters such that the chosen method results in the desired crystals.

One preferred method of crystallization of ZAP-70 involves mixing a ZAP-70 solution with a "reservoir buffer", with a lower concentration of the precipitating agent necessary for crystal formation. For crystal formation, the concentration of the precipitating agent has to be increased, e.g. by addition of precipitating agent, for example by titration, or by allowing the concentration of precipitating agent to balance by diffusion between the crystallization buffer and a reservoir buffer. Under suitable conditions such diffusion of precipitating agent occurs along the gradient of precipitating agent, e.g. from the reservoir buffer having a higher concentration of precipitating agent into the crystallization buffer having a lower concentration of precipitating agent. Diffusion may be achieved e.g. by vapour diffusion techniques allowing diffusion of water in the common gas phase. Known techniques are e.g. vapour diffusion methods, such as the "hanging drop" or the "sitting drop" method. In the vapour diffusion method a drop of crystallization buffer containing the protein is hanging above or sitting beside a much larger pool of reservoir buffer. Alternatively, the balancing of the precipitating agent can be achieved through a semipermeable membrane that separates the crystallization buffer from the reservoir buffer and prevents dilution of the protein into the reservoir buffer.

Formation of ZAP-70 kinase catalytic domain crystals can be achieved under various conditions which are essentially determined by the following parameters: pH, presence of salts and additives, precipitating agent, protein concentration and temperature. The pH may range, for example, from about 4.0 to 9.0.

The present invention also relates to a computer readable medium having stored a model of the ZAP-70 catalytic domain crystal structure. In a preferred embodiment, said model is built from all or part of the X-ray diffraction data shown in the atomic coordinates of Table 1.

The present invention provides the structure coordinates of human ZAP-70 catalytic domain. The term "structure coordinates" or "atomic coordinates" refers to mathematical coordinates derived from the mathematical equations related to the pattern obtained on diffraction of a monochromatic beam of X-rays by the atoms (scattering centers) of a crystal comprising a

ZAP-70 catalytic domain. The diffraction data are used to calculate an electron density map of the repeating unit of the crystal. The electron density maps are used to establish the positions of the individual atoms within the unit cell of the crystal.

Structural coordinates of a crystalline composition of this invention may be stored in a machine-readable form on a machine-readable storage medium, e.g. a computer hard drive, diskette, DAT tape, etc., for display as a three-dimensional shape or for other uses involving computer-assisted manipulation of, or computation based on, the structural coordinates or the three-dimensional structures they define. For example, data defining the three dimensional structure of a protein of the ZAP family, or portions or structurally similar homologues of such proteins, may be stored in a machine-readable storage medium, and may be displayed as a graphical three-dimensional representation of the protein structure, typically using a computer capable of reading the data from said storage medium and programmed with instructions for creating the representation from such data.

In one embodiment of the invention, a method is provided for determining the three-dimensional structure of the catalytic domain of ZAP-70 comprising:
(i) crystallization of ZAP-70 kinase comprising the catalytic domain of ZAP-70 (SEQ ID No.2), fragment or homologue thereof
(ii) collecting x-ray diffraction data in the form of atomic coordinates for said crystal
(iii) utilizing the atomic coordinates of Table 1 in whole or in part to determine the three-dimensional structure of the catalytic domain of ZAP-70, fragment, or homologue thereof.

In another embodiment of the invention, a method is provided for determining the three-dimensional structure of a complex comprising the catalytic domain of ZAP-70 kinase (SEQ ID No.2), fragment or homologue thereof bound to at least one ligand comprising:
(i) obtaining x-ray diffraction data for a crystal of the complex
(ii) utilizing the atomic coordinates of Table 1 in whole or in part to determine the three-dimensional structure of the complex.

According to the present invention, a three-dimensional ZAP-70 model is obtainable from a ZAP-70 crystal comprising the catalytic domain of ZAP-70, fragment or homologue thereof. Such a model can be built or refined from all or part of the ZAP-70 kinase structure data of

the present invention using the x-ray diffraction coordinates, particularly the atomic structure coordinates of Table 1.

The knowledge obtained from the three-dimensional model of the catalytic binding site of ZAP-70 can be used in various ways. For example, it can be used to identify chemical entities, for example, small organic and bioorganic molecules such as peptidomimetics and synthetic organic molecules that bind to ZAP-70 and preferably block or prevent a ZAP-70 mediated or associated process or event, or that act as ZAP-70 agonists. Using the three-dimensional structure of the ZAP-70 catalytic domain, the skilled artisan constructs a model of the ZAP-70. For example, every atom can be depicted as a sphere of the appropriate van der Waals radius, and a detailed surface map of the ZAP-70 catalytic domain can be constructed.

Chemical entities that have a surface that mimics the accessible surface of the catalytic binding site of ZAP-70 can be constructed by those skilled in the art. By way of example, the skilled artisan can screen three-dimensional structural databases of compounds to identify those compounds that position appropriate functional groups in similar three dimensional structural arrangement, then build combinatorial chemistry libraries around such chemical entities to identify those with high affinity to the catalytic binding site of ZAP-70.

In one embodiment of the invention, a method is provided for identifying a ligand or low molecular weight compound that binds to the catalytic domain of ZAP-70 kinase comprising the steps of:
(i) using the three-dimensional structure of the catalytic domain derived in whole or in part from the set of atomic coordinates in Table 1 to select a potential ligand or low molecular weigh compound that binds to the catalytic domain of ZAP-70
(ii) selecting those ligands or low molecular weight compounds that bind to the catalytic domain of ZAP-70.

In another embodiment of the invention, a method is provided for identifying a ligand or low molecular weight compound that binds to the catalytic domain of ZAP-70 kinase wherein the catalytic domain of ZAP-70 comprises at least the ATP binding site of said domain.

In yet another embodiment of the invention, a method is provided for identifying ligands which inhibit the biological activity of ZAP-70 kinase.

Ligands or small molecular compounds can be identified from screening compound databases or libraries and using a computational means to form a fitting operation to a binding site on the catalytic domain of ZAP-70 kinase. The three dimensional structure of the catalytic domain of ZAP-70 as provided in the present invention in whole or in part by the structural coordinates of Table 1, can be used together with various docking programs.

The potential inhibitory or binding effect of a chemical entity on ZAP-70 may be analyzed prior to its actual synthesis and testing by the use of computer-modeling techniques. If the theoretical structure of the given chemical entity suggests insufficient interaction and association between it and ZAP-70, the need for synthesis and testing of the chemical entity is obviated. However, if computer modeling indicates a strong interaction, the molecule may then be synthesized and tested for its ability to bind to ZAP-70. Thus, expensive and time-consuming synthesis of inoperative compounds may be avoided.

An inhibitory or other binding compound of ZAP-70 may be computationally evaluated and designed by means of a series of steps in which chemical entities or fragments are screened and selected for their ability to associate with the individual binding sites of ZAP-70. Thus, one skilled in the art may use one of several methods to screen chemical entities or fragments for their ability to associate with ZAP-70. This process may begin by visual inspection of, for example, the binding site on a computer screen based on the structural coordinates of Table 1 in whole or in part. Selected fragments or chemical entities may then be positioned in a variety of orientations, or "docked," within the catalytic binding site of ZAP-70. Docking may be accomplished using software such as Quanta and SyLyl, followed by energy minimization and molecular dynamics with standard molecular mechanics force fields, such as CHARMM and AMBER. Specialized computer programs may be of use for selecting interesting fragments or chemical entities. These programs include, for example, GRID, available from Oxford University, Oxford, UK; 5 MCSS or CATALYST, available from Molecular Simulations, Burlington, MA; AUTODOCK, available from Scripps Research Institute, La Jolla, CA; DOCK, available from University of California, San Francisco, CA, and XSITE, available from University College of London, UK.

Using molecular replacement to exploit a set of coordinates such as those of Table 1 of the invention, the structure of a crystalline ZAP-kinase catalytic domain or portion thereof can for example, be bound to one or more ligands or low molecular weight compounds to form a complex.

The term "molecular replacement" refers to a method that involves generating a preliminary structural model of a crystal whose structural coordinates are unknown, by orienting and positioning a molecule whose structural coordinates are known, e.g., the ZAP-70 kinase catalytic domain coordinates within the unit cell of the unknown crystal, so as to best account for the observed diffraction pattern of the unknown crystal. Phases can then be calculated from this model, and combined with the observed amplitudes to give an approximated Fourier synthesis of the structure whose coordinates are unknown. This in turn can be subject to any of the several forms of refinement to provide a final accurate structure of the unknown crystal. Using the structural coordinates provided by this invention, molecular replacement may be used to determine the structural coordinates of a crystalline co complex, unknown ligand, mutant, or homolog, or of a different crystalline form of ZAP-70 kinase. Additionally, the claimed crystal and its coordinates may be used to determine the structural coordinates of a chemical entity that associates with ZAP-70.

"Homology modeling" according to the invention involves constructing a model of an unknown structure using structural coordinates of one or more related proteins, protein domains and/or one subdomains such as the catalytic domain of ZAP-70 kinase. Homology modeling may be conducted by fitting common or homologous portions of the protein or peptide whose three dimensional structure is to be solved to the three dimensional structure of homologous structural elements. Homology modeling can include rebuilding part or all of a three dimensional structure with replace of amino acids or other components by those of the related structure to be solved.

Molecular replacement according to the present invention, uses a molecule having a known structure. The three-dimensional structure of the catalytic domain of ZAP-70 provided in whole or in part in Table 1 in a machine-readable form on a data-carrier can be used as a starting point to model the structure of an unknown crystalline sample. This technique is based on the principle that two molecules which have similar structures, orientations and positions in the unit cell diffract similarly. Molecular replacement involves positioning the

known structure in the unit cell in the same location and orientation as the unknown structure. Once positioned, the atoms of the known structure in the unit cell are used to calculate the structure factors that would result from a hypothetical diffraction experiment. This involves rotating the known structure in the six dimensions (three angular and three spatial dimensions) until alignment of the known structure with the experimental data is achieved. This approximate structure can be fine-tuned to yield a more accurate and often higher resolution structure using various refinement techniques. For instance, the resultant model for the structure defined by the experimental data may be subjected to rigid body refinement in which the model is subjected to limited additional rotation in the six dimensions yielding positioning shifts of under about 5%. The refined model may then be further refined using other known refinement methods. The present invention also enables homologues and mutants of ZAP-70 catalytic domain and the solving of their crystal structure. Based on the three-dimensional structure of ZAP-70 catalytic domain as provided in the present invention and using the atomic coordinates of Table 1 in whole or in part, the effects of site-specific mutations can be predicted. More specifically, the structural information provided herein permits the identification of desirable sites for amino acid modification, particularly amino acid mutation resulting in substitutional, insertional or deletional variants. Such variants may be designed to have special properties, particularly properties distinct from wild-type ZAP-70 catalytic domain, such as altered catalytic activity. Substitutions, deletions and insertions may be combined to arrive at a desired variant. Such variants can be prepared by methods well-known in the art, e.g. starting from wild-type ZAP-70 catalytic domain, or by de novo synthesis.).

ZAP-70 catalytic domain may also crystallize in a form different from the one disclosed herein. The structural information provided, for example, in SEQ ID No. 2 and Table 1 in whole or in part, is also useful for solving the structure of other crystal forms. Furthermore, it may serve to solve the structure of a ZAP-70 catalytic domain mutant, a ZAP-70 catalytic domain co-complex or a sufficiently homologous protein.

The ZAP-70 catalytic domain structural information provided herein is useful for the design of ligands or small molecule compounds which are capable of selectively interacting with ZAP-70 catalytic domain and thereby specifically modulating the biological activity of ZAP-70. Furthermore, this information can be used to design and prepare ZAP-70 mutants, e.g. mutants with altered catalytic activity, model the three-dimensional structure and solve the

crystal structure of proteins, such as ZAP-70 catalytic domain homologues, ZAP-70 catalytic domain mutants or ZAP-70 catalytic domain co-complexes, involving e.g. molecular replacement.

The present invention provides a method for designing a ligand or low molecular weight compound capable of binding with ZAP-70 catalytic domain, said method comprising:

(i) using the atomic coordinates of Table 1 in whole or in part to determine the three-dimensional structure of the ZAP-70 catalytic domain

(ii) probing said three-dimensional structural of the ZAP-70 catalytic domain with candidate ligands or low molecular weight compounds to determine which bind to the catalytic domain of ZAP-70

(iii) selecting those ligands or low molecular weight compounds which bind to the catalytic domain of ZAP-70

(iv) optionally, modifying those ligands or low molecular weight compounds which bind to maximize physical binding properties such as solubility, affinity, specificity or potency.

Preferred is a method for designing a ZAP-70 inhibitor which interacts at the catalytic binding site. The present invention also relates to the chemical entity or ligand identified by such method. One approach enabled by this invention is the use of the structural coordinates of ZAP-70 catalytic domain to design chemical entities that bind to or associate with ZAP-70 kinase and alter the physical properties of the chemical entities in different ways. Thus, properties such as, for example, solubility, affinity, specificity, potency, on/off rates, or other binding characteristics may all be altered and/or maximized. One may design desired chemical entities by probing an ZAP-70 crystal comprising the catalytic domain with a library of different entities to determine optimal sites for interaction between candidate chemical entities and ZAP-70. For example, high-resolution x-ray diffraction data collected from crystals saturated with solvent allows the determination of where each type of solvent molecule adheres. Small molecules that bind tightly to those sites can then be designed and synthesized and tested for the desired activity. Once the desired activity is obtained, the molecules can be further altered to maximize desirable properties.

The invention also contemplates computational screening of small-molecule databases or designing of chemical entities that can bind in whole or in part to ZAP-70 catalytic domain. They may also be used to solve the crystal structure of mutants, co-complexes, or the

crystalline form of any other molecule homologous to, or capable of associating with, at least a portion of ZAP-kinase. One method that may be employed for this purpose is molecular replacement. An unknown crystal structure, which may be any unknown structure, such as, for example, another crystal form of ZAP-70 kinase catalytic domain, an ZAP-70 kinase catalytic domain mutant or peptide, or a co-complex with ZAP-70 kinase, or any other unknown crystal of a chemical entity that associates with ZAP-70 that is of interest, may be determined using the whole of part of the structural coordinates set forth in Table 1. This method provides an accurate structural form for the unknown crystal far more quickly and efficiently than attempting to determine such information without the invention herein.

In one preferred embodiment of the invention, candidate ligands are screened in silico. The information obtained can thus be used to obtain maximally effective inhibitors or agonists of ZAP-70. The design of chemical entities that inhibit or agonize ZAP-70 generally involves consideration of at least two factors. First, the chemical entity must be capable of physically or structurally associating with ZAP-70, preferably at the catalytic site of ZAP-70. The association may be any physical, structural, or chemical association, such as, for example, covalent or noncovalent bonding, or van der Waals, hydrophobic, or electrostatic interactions. Second, the chemical entity must be able to assume a conformation that allows it to associate with ZAP-70, preferentially at the catalytic site of ZAP-70. Although not all portions of the chemical entity will necessarily participate in the association with ZAP-70, those non-participating portions may still influence the overall conformation of the molecule. This in turn may have a significant impact on the desirability of the chemical entity. Such confirmational requirements include the overall three-dimensional structure and orientation of the chemical entity in relation to all or a portion of the binding site.

Once a compound has been designed or selected by the above methods, the efficiency with which that compound may bind to ZAP-70 may be tested and modified for the maximum desired characteristic(s) using computational or experimental evaluation. Various parameters can be maximized depending on the desired result. These include, but are not limited to, specificity,affinity, on/off rates, hydrophobicity, solubility, and other characteristics readily identifiable by the skilled artisan.

The present invention also relates to identification of compounds which modulate ZAP-70. Preferred are compounds which inhibit ZAP-70 activity and are potentially useful for the

treatment of diseases and conditions such as those which involve T cell and lymphocyte activation.

The present invention enables the use of molecular design techniques, particularly the rational drug design approach, to prepare new or improved chemical entities and compounds, including ZAP-70 inhibitors, capable of irreversibly or reversibly, modulating ZAP-70 activity. Improved entities or compounds means that these entities or compounds are superior to the "original" or parent compound they are derived from with regard to a property relevant to therapeutic use including suitability for in vivo administration, e.g. cellular uptake, solubility, stability against (enzymatic) degradation, binding affinity or specificity, and the like. For example, on the basis on the information provided herein it is possible to specially design ZAP-70 inhibitors which covalently, or preferably non-covalently, bind to ZAP-70. Such inhibitors may act in a competitive or uncompetitive manner, bind at or close to the active site of ZAP-70 or act allosterically.

In the design of ZAP-70 modulators the following aspects should be considered: (i) if the candidate compound is capable of physically and structurally associating with ZAP-70 kinase catalytic domain, and/or (ii) if the compound is capable of assuming a conformation allowing it to associate with ZAP-kinase catalytic domain. Advantageously, computer modelling techniques are used in the process of assessing these abilities for the modulator as a whole, or a fragment thereof - in order to minimize efforts in the synthesis or testing of insuccessful candidate compounds. Specialized computer software is well-known in the art.

Another design approach is to probe a ZAP-70 catalytic domain crystal with a variety of different chemical entities to determine optimal sites for interaction beween candidate ZAP-70 inhibitors and the target enzyme. Yet another possibility which arises from the present invention is to screen computationally small molecule data bases for chemical entities or compounds that are capable of binding, in whole or in part, to ZAP-70 catalytic domain. The quality of fit to the binding site may be judged e.g. by shape complementarity or by estimated interaction energy. Knowledge of the three-dimensional arrangement of the modifications can be then utilized for the design of new ZAP-70 ligands or low molecular weight compounds such as selective inhibitors.

Chemical entities that are capable of associating with the ZAP family member may inhibit its interaction with naturally occurring ligands of the protein and may inhibit biological functions mediated by such interaction. In the case of ZAP-70, such biological functions include activation of T cells during an immune response. Such chemical entities are potential drug candidates.

Compounds of the structures selected or designed by any of the foregoing means may be tested for their ability to bind to a ZAP family protein, inhibit the binding of a ZAP family protein to a natural or non-natural ligand therefor, and/or inhibit a biological function mediated by a ZAP family member.

The following examples serve to illustrate the present invention but should not be construed as a limitation thereof. The invention particularly relates to the specific embodiments described in these examples. Compounds first identified by any of the methods described herein are also encompassed by this invention.

Examples

Example 1: Initial Purification of Full-Length ZAP kinase

The full length amino acid sequence of the ZAP-70 kinase is given in SEQ ID No. 1. N-terminally His$_6$-tagged full-length ZAP kinase is expressed in Sf9 cells, this differs from the wild-type sequence in that the N-terminal is modified by insertion of a hexa-histidine sequence in between the N-terminal methionine and proline (position 2), such that this proline is now in position 8. Cell pellets are harvested and frozen at –80°C until required. A 39g wet cell pellet is suspended in 350ml ice-cold buffer A (50mM sodium phosphate pH 8, containing 12 EDTA-free Complete™ protease inhibitor tablets, 10mM β-mercaptoethanol, 10% v/v glycerol, 0.1mM MnCl$_2$, 10mM imidazole and 300mM NaCl). The cells are lysed for 3 minutes on ice using a Heidolph-Diax tissue-grinder followed by 10 strokes in a glass-teflon homogeniser. The resultant lysate is centrifuged for 45 min at 43,000g at 4°C and subsequently filtered through successive glass-fibre, 1.2µM and 0.43µM filter membranes. This clarified supernatant is loaded at a flow-rate of 2ml/min onto an XK16/20 chromatography column (Amersham Biosciences) containing 20ml Ni-NTA-agarose (Qiagen) affinity resin equilibrated with buffer A. Once all the material has been loaded, the column is washed (at a flow-rate of 4ml/min) with buffer A until the UV-absorbance of the

flow-through material has once again returned to baseline levels. At this point (using the same flow-rate), buffer B (25mM Tris-HCl pH8, 10% v/v glycerol, 50mM NaCl and 250mM imidazole) is applied to the column and the peak of protein which elutes is collected. This material is loaded directly onto a 16ml column of γ-aminophenyl-ATP sepharose equilibrated with buffer C (25mM Tris pH 8.0 containing: 30% v/v glycerol, 1mM DTT, 1mM MgCl$_2$ and 50mM NaCl) at a flow-rate of 2ml/min. The column is eluted by applying a gradient of 0 - 1M NaCl in buffer C over 7 column volumes. The eluted peak is concentrated by ultrafiltration using a 30,000 M$_r$ cut-off membrane (Amicon) to approximately 7ml and further purified using a Superdex 75 (XK16/60) size-exclusion column equilibrated with buffer C (but without 50mM NaCl). The fractions containing ZAP 70 monomer are collected and pooled prior to concentration to 2.5mg/ml and subsequent limited proteolytic digestion.

Full-length ZAP-70 is eluted from the NTA-agarose column at a purity of approximately 60% as determined by reducing SDS-PAGE. Subsequent chromatography on a 16ml column of γ-aminophenyl-ATP sepharose gives a rather broad peak of much higher purity which can be concentrated. Detailed analysis of this peak reveals that the earlier eluting fractions contain predominantly aggregated material and that a discrete peak towards the end of the profile contains most of the monomeric ZAP of high purity. Size-exclusion chromatography gives a major peak comprising ~90% of the protein, the remainder eluting slightly earlier in a position where dimeric or aggregated protein would be expected to elute. At this stage the purity of the preparation is in excess of 90% and suitable for use in the limited proteolytic definition of minimal kinase domains. At this stage, highest purity is very important so as to minimise the number of additional sequences present following proteolytic digestion.

Example 2: Proteolytic catalytic domain definition

ZAP-70 is incubated for 20h at room temperature at a 1:100 concentration ratio with the following proteases: thermolysin, carboxypeptidase A, thrombin, Arg C, Glu C, Factor Xa, Carboxypeptidase Y, chymotrpsin, Lys C, Asp N, elastase, trypsin and subtilisin (1:1 ratio). Following incubation samples are removed, subjected to reducing SDS-PAGE electrophoresis (Novex 4-20% gels, Invitrogen) and compared with non-digested controls. In the cases where faster migrating bands are observed, which are of sufficient size (~30 kDa) to contain the catalytic domain, samples are re-run on SDS-PAGE and Western-blotted using an anti-His$_6$ antibody (Sigma, H-1029). This is in order to identify N-terminal and C-terminal ZAP-70 fragments (the His$_6$-tag is at the N-terminus, consequently forms showing

anti-His$_6$ immunoreactivity are truncated at the C-terminus and are of no interest). Non-immunoreactive fragments are subjected to SDS-PAGE and transferred electrophoretically to PVDF membranes, the bands visualised, excised and their N-terminal sequences analysed.

Following digestion with thermolysin, trypsin, Glu C, Asp N and elastase, faster migrating bands are observed which are of sufficient size (~30 kDa) to contain the catalytic domain. When Western-blotted against the (His)$_6$ N-terminal tag, non-immunoreactive fragments are produced by trypsin, elastase and thermolysin digestion, and are thereby defined as being C-terminal in origin. These fragments are sequenced. Trypsin and Thermolysin digestion both give a fragment with Isoleucine 299 as N-terminus. Elastase produces an arginine298 fragment and thermolysin an additional leucine277 fragment. Based upon these results, ZAP catalytic domains beginning with leucine277 and arginine298 are identified as being potentially suitable for crystallisation.

Example 3: Cloning of PreScission™ I and II constructs

Previous attempts to purify a number of catalytic domain constructs proved difficult due to low levels of expression of soluble protein and instability of these proteins. This instability might be, in part, due to incorrect *in-vivo* folding of the isolated domains and in part due to non-optimal construct length.Therefore, the full-length ZAP-70 is expressed, flanked by the PreScission™ protease recognition sequences to facilitate efficient proteolytic release of the desired domain. Based on the results obtained from the limited proteolysis of the full-length version of ZAP-70, two constructs were made: PreScission™ I, a C-terminally His$_6$-tagged ZAP-70 with a PreScission site inserted immediately prior to leucine 277 (residue 285 in construct) and PreScission II™, which contained two such sites, one upstream of arginine298 (residue 306 in construct) and one upstream of the C-terminal His$_6$ tag, so that this could be removed simultaneously . With the oligonucleotide MG474 and RS366 (see: SEQ ID No.3 and 4 respectively) and the plasmid NPL2173 encoding the wild type full-length ZAP-70 gene (Genbank Accession Nr. L05148), a DNA fragment is amplified which upon integration into the original NPL2173 allows the introduction of the PreScission™ cleavage site between alanine297 and arginine298. Another cleavage site is added after alanine619, preceeding the (His)$_6$-tag. The integration of the PCR fragment is done as described earlier (Geiser et al. Biotechnology 2001). The resulting plasmid is sequenced and the correct clone called pXI347 (PlasNova NPL003792). Similarly the plasmid pXI345 (NPL003793) is

constructed by integrating the PCR fragment obtained from the NPL2173 plasmid template with the oligonucleotides MG475 and MG479 (SEQ ID No 5 and SEQ ID No 6) In pXI345, the PreScission™ cleavage site is integrated between threonine282 and leucine277 and the PreScission™ cleavage site in front of the (His)₆-tag is removed. The two plasmids are then introduced by transfection together with a linearized baculovirus DNA into insect cells. The numbering of amino acids is based on the sequences differs from that of Genbank Accession number L05148, by virtue of the inclusion of the purification tag and the inserted protease recognition sequences.

Based on the results of the limited proteolysis of the full sized ZAP-70 introduced after positions 276, 297 and after amino acid position 619, PreScission™ cleavage sites. The plasmids encoding the new mutants of ZAP-70 are called pXI345 and pXI347 respectively. These plasmids encode the protein ZAP PreScission™ I and ZAP PreScission™ II respectively. As a result of the mutations, complete and highly specific proteolysis of the full-length proteins can be carried out with a high quantitative recovery of the catalytic domain of ZAP-70.

Example 4: Expression and medium-scale fermentation of PreScission II ZAP in Baculovirus

Sf21 cells propagated in Excell 401 medium with 10 % fetal calf serum are transfected with 500 ng of each recombinant transfer vector and 5 µl of linear AcNPV virus DNA (BacPAK 6) by lipofection using Bacfectin as transfection reagent (both BD/Clontech, Palo Alto, Ca.). After five days of incubation, the transfection supernatants are harvested and subjected to plaque assay, to derive a homogenous viral population. The isolated virus plaque picks are further amplified by infection of Sf21 cells grown in suspension in Excell 401 plus 1 % FCS in roller culture, until full working virus stocks of both viruses are developed. These are again titered by plaque assays.

Large scale productions are carried out using the Wave bioreactor (Wave Biotech AG, Tagelswangen, Switzerland) at 10 l working volume. Sf9 cells growing in SF900 II medium (Gibco/Life Technologies) are inoculated in the Wave bag and allowed to grow for three consecutive days, reaching maximal cell densities of approx. 5 x 10⁶ cells ml. During the cultivation and infection process the airflow, the rocking rate and the rocking angle of the Wave reactor thermoplate are monitored and adjusted. The Sf9 cells are infected at cell

densities of 1.6-4.9 x 10^6 cells/ml and different multiplicities of infection (m.o.i.) between 0.5, 1 and 2 m.o.i.. Simultaneously with virus addition, yeastolate (Gibco/Life Technologies) is fed to the cultures at a final concentration of 4 g/l. Cell density as well as cell viability is carefully recorded during the infection period.

Plaque assays of the amplified working virus stocks give rise to titers of 5.6 x 10^7 pfu/ml for the ZAP70 PreScission™ I construct and 1.7 x 10^8 pfu/ml for the ZAP-70 PreScission™ II construct. Both are subsequently used for 10 litre large-scale production of the two PreScission™ ZAP constructs. Both proteins are well-expressed and at least partially soluble; however, although LC-MS of NTA superflow purified PreScission™ II showed several peaks with masses of 72,404, 72,478, 72,557 and 72,635 which were thought to correspond to non-, mono-, di- and tri-phosphorylated full-length kinase, the PreScission™ I material gave such a heterogeneous LC-MS spectrum that it was impossible to assign masses, therefore all expression efforts were concentrated towards production of the PreScission™ II construct.

Example 5: Method for optimising harvesting of the Sf9 cultures

The baculovirus expression system is a lytic system; as the infection proceeds, cells die and lyse, losing their contents into the medium. In the case of the expression of proteins such as ZAP, which are expressed intracellularly, there is a small "window" of expression in which maximal protein expression occurs before this is lost through cell lysis. Typically Western blotting will be used in conjunction with a time course of infection as well as variation of the multiplicity of infection (m.o.i.) to determine this time-point. However, in the case of ZAP PreScission™ II, the observation is made that increasing levels of expression are also accompanied by increasing levels of insoluble protein. Therefore, rapid small-scale purifications lysing 1g quantities of cells give an "on-line" readout of "purifiable" ZAP.

1g cell pellets are removed at different time points during fermentation and lysed as described previously (but using 15ml lysis buffer, containing 1 Complete™ EDTA-free protease inhibitor tablet). Due to the scale-down, a 0.5ml Ni-NTA-agarose column is used and the whole process from lysis through to analytical RP-HPLC estimate of the content of isolated protein is reduced to 3-4 hours. With an optimised harvest time of 48 h, the yield of soluble ZAP can be increased 4-fold to approximately 0.75mg purifiable ZAP/g cells or ~7.5mg/litre culture.

Example 6: Staurosporin binding to the ZAP kinase catalytic domain

ZAP-70 kinase catalytic domain (R_{298}- A_{619}; SEQ ID No.2) defined by limited proteolysis is recloned as the full-length ZAP-70 kinase with a C-terminal His_6-affinity tag, but flanked by two PreScission™ protease sites. Expression is carried out using SF9 cells grown in 10 litre Wave™ bioreactors (0.45 m.o.i; 48 h). Cells are lysed in ice-cold buffer A (50mM $NaPO_4$, 10% v/v glycerol, 10mM β-mercaptoethanol, 300mM NaCl, 10mM Imidazole; pH 8.0) containing Complete™ EDTA-free protease inhibitor. The clarified lysate is passed over a 20ml Ni-NTA-agarose column, the column washed with buffer A and then eluted with buffer B (25mM Tris, 10% v/v glycerol, 50mM NaCl, 250mM Imidazole; pH 8.0). All chromatography steps are either carried out on-ice or using jacketed, cooled columns. The protein is immediately desalted into 25mM Tris pH8.0, containing 1mM EDTA, 1mM DTT, 30%v/v glycerol and 150mM NaCl, (using a 50ml sephadex G-25 desalting column; HiPrep™ 26/10 Amersham Biosciences) concentrated and staurosporin added to 2-Molar excess (by addition of the correct volume of staurosporin dissolved in DMSO to 2mg/ml).

The protein solution (60ml) is frozen at –80 °C until required then concentrated using a 30,000 M_r cut-off ultrafiltration membrane (Amicon) down to 10-15ml prior to size-exclusion chromatography using an XK26/90 column packed with Superdex 75™ and equilibrated with 25mM Tris pH 8, 1mM EDTA, 1mM DTT, 150mM NaCl and 30% v/v glycerol. Fractions are collected, those corresponding to the monomeric material (ca. 40ml) are pooled and incubated with PreScission™ protease to excise the catalytic domain from the rest of the molecule. Typically 40ml of solution, containing 42mg ZAP PreScission™ II is digested for 135 min at room temperature with 420µl PreScission™ protease solution. The cleavage reaction is monitored by reversed phase HPLC so that the reaction can be stopped as quickly as possible by immediately desalting into buffer C (20mM $NaPO_4$, 5mM DTT, 10mM NaCl, 1mM $MgCl_2$: pH 7.2). Typically as 3 x 14ml portions, applied at a flow-rate of 5ml/minute to a HiLoad™ 26/10 column. The desalted protein, containing a mixture of monophosphorylated (25%) and non-phosphorylated (75%) ZAP is applied to an HR10/8 cation-exchange column (Mono S™ Amersham Biosciences) equilibrated in buffer C. The column is loaded at a flow-rate of 1ml/minute and eluted at two ml/min using a 0-250mM NaCl gradient over 512ml.

Two major peaks are eluted, the monophosphorylated protein eluting at approximately 80mM NaCl, the non-phosphorylated protein, slightly later at approximately 100mM NaCl.

The non- and mono-phosphorylated ZAP kinase catalytic domain peaks are collected separately, desalted (HiLoad 26/10 column) into 20mM HEPES pH 7.2 (containing 5mM DTT, 1mM MgCl$_2$, 150mM NaCl and 1% v/v ethyleneglycol). Staurosporine is again added to 10 Molar excess to both forms which are subsequently concentrated to 10-40 mg/ml for crystallisation. This desalting step is critical, because it removes the glycerol required for chromatography (without which, the protein precipitates) and replaces it with a low concentration of ethylene glycol which sufficiently stabilises the protein through the concentration step, but doesn't interfere with the subsequent crystallization. 30% v/v glycerol, on the other hand, is not suitable for crystallisation as it has too large an influence on the evaporative sitting-drop process. In the case of the non-phosphorylated protein, half of the eluted peak, 36ml is concentrated to 130μl and a final concentration of 36mg/ml.

By optimisation of the fermentation and harvest conditions, the level of ZAP expression is increased such that the purity of ZAP PreScission™ II being eluted from the NTA column is in excess of 75% and could be adequately purified by an additional size-exclusion chromatography step prior to cleavage. Following cleavage with PreScission™ protease, two bands are observed of similar mass representing the kinase and N-terminal portions of the molecule. Cation-exchange chromatography is applied to separate the two forms. The N-terminal portion passed through the column under the conditions used. The two peaks that are eluted from the column represented two different phosphorylated forms; the monophosphorylated protein eluting at approximately 80mM NaCl and the non-phosphorylated protein, slightly later at approximately 100mM NaCl. These different forms are collected separately for crystallisation. The yield of the mono-phosphorylated form is approximately 4-fold lower than the non-phosphorylated form, therefore most crystallography efforts concentrated on the non-phosphorylated form.

Example 7: Crystallisation of PreScission II ZAP

9 mg/ml ZAP-70 non-phosphorylated catalytic kinase domain in 20 mM Hepes, 5 mM DTT, 1 mM MgCl$_2$, 150 mM NaCl, 30 % Glycerol, and staurosporine, are used for initial crystallization screening using 96 well sitting drop crystallography plates. The first promising microcrystals are obtained with crystallization screen at 10° C. Optimization of these crystallisation conditions is carried out by hanging drop vapor diffusion. The crystallisation screen at 10° C has the following crystallisation conditions: 0.1 M Tris pH 7.5, 0.1 M KCl, 18 % PEG 5000 monomethylether. Optimisation of this crystallisation condition along with

optimisation of the formulation of the protein preparation results in larger crystals. Hanging drop vapor diffusion is used for optimisation. Diffracting single crystals are obtained with 29 mg/ml Zap70 nonphosphorylated kinase domain in 20 mM Hepes, 5 mM DTT, 1 mM MgCl$_2$, 150 mM NaCl, 1% Ethylene glycol, and staurosporine. The optimal growth condition is: 0.1 M Tris HCl pH 7.5, 0.2 M KCl, 20 % PEG 5000 monomethylether at a crystallisation temperature of 10° C. Crystals appear after 1-2 days and optimal crystal size is reached after 1-2 weeks. Some single crystals grow, but most single fragments are obtained by breaking apart clusters.

Example 8: Protein production and crystallization of the Human ZAP-70 protein kinase catalytic domain

SEQ ID No.2 of the human ZAP-70 protein kinase catalytic domain (non-phosphorylated) is used for crystallization The construct comprises ZAP-70 residues 298 to 619 plus two additional residues from the PreScission™ cleavage site at the N-terminus and 6 residues from the PreScission™ cleavage site at the C-terminus. Small, but well-diffracting single crystals are obtained with a preparation of 29 mg/ml protein concentration and 1 % Ethylene glycol. Optimal growth conditions are 20 % PEG 5000 monomethylether, 0.1 M Tris HCl pH 7.5, 200 mM KCl. Crystals appear after 1-2 days and optimal crystal size is reached after 1-2 weeks. Some single crystals form but most single fragments are obtained by breaking apart clusters.

Cryo-protection

Crystals are transferred from the drop into a solution consisting of the crystallization solution (well solution) plus 20% (v/v) of glycerol and 1 mM inhibitor. Crystals mounted in a 0.05 µm cryo loop are soaked in this cryo buffer for about 10-15 sec and then dipped into liquid propane.

Data collection

A crystal is frozen in liquid propane and diffraction data are collected at 80K with a MAR CCD camera at the SLS in Villingen, Switzerland. A wavelength of 0.9803 A is used. 340 images are collected with 1.0° oscillation each, using an exposure time of 6sec per frame and a crystal-to-detector distance of 140mm. Raw diffraction data are processed and scaled with the HKL program suite version 1.96.6 (Otwinowski and Minor, 1996). Crystal data and data statistics are shown in Table 2.

Structure determination and refinement

The structure of the catalytic Zap70 kinase domain is determined by molecular replacement, using the coordinates of the LCK kinase domain x-ray structure (pdb: 3LCK, Yamaguchi and Hendrickson, 1996) as search model. Residues 245 to 501 of LCK are used and the phospho-Tyr residue 394 is removed for sequence similarity comparisons.

Molecular replacement is performed with the auto molecular replacement script in CCP4, using data to a maximal resolution of 4.0 Å. A 80% fraction completeness of the model with 50% fraction similarity to the input structure and 2 molecules in the asymmetric unit is expected. A clear solution is found and after an initial refinement in CNX using the standard script refine.inp the structure has an R-factor of 41.7 % (R-free 43.5%). Inspection of the σ_A-weighted Fo-Fc electron density map with the program O version 7.0 (Jones et al., 1991) reveals a strong density for most of the C-alpha trace and most of the side chains. There are several insertions and deletions and a number of loops which are found outside the electron density and have to be corrected manually.

The model of the human ZAP-70 protein kinase catalytic domain is built and adjusted to fit the density where necessary. Insertions, mutations and deletions are made accordingly. The numbering was changed using the numbering of the SwissProt Accession number P43403 entry for ZAP-70. The structure is refined by a number of cycles of torsion angle dynamics and energy minimization, interspersed by model rebuilding steps. For refinement, the "refine.inp" script of CNX 2000 is used, with the following (non-default) option: Bulk solvent correction (based on the mask method).

Cross-validation is used throughout refinement using a test set comprising 5% of the reflections. Water molecules are identified with the CNX script water_pick.inp, and selected based on difference peak height (greater than 3.0σ), hydrogen-bonding and distance criteria. NCS restrain is used for the two molecules in the asymmetric unit.

The quality of the final refined model is assessed with the programs CNX 2000 (Brünger, 1998) (see: Figure 7). Pictures are made in O (Jones et al., 1991) or WebLab ViewerLite 3.5 (Molecular Simulations, Inc.).

Results

Small single crystals of the human Zap70 kinase domain are obtained with PEGMME at pH 7.5. The crystals grow in space group P1 with 2 monomers per asymmetric unit. The

structure is determined by molecular replacement. The final model includes two kinase domains (residue 331 to 603), one molecule of staurosporine per kinase domain and 261 water molecules. It has a good geometry with a rms deviation of 0.011 Å on bond lengths and 1.3° on bond angles. The final R-factor was 0.182 (Rfree= 0.209) for all reflections between 19.26 Å and 1.90 Å.

Overall structure

The crystal structure is extremely well defined, the full c-alpha trace between residue 331 and 603 is defined. All loops and important residues have good electron density. The B-factor distribution is as expected. The staurosporine-binding site and all interactions with the kinase domain can be described in detail. The quality of the model is good, the final R-factor is 18.2% (R-free 20.9%).

The ZAP-70 kinase domain folds into the typical kinase domain fold. Most of the residues are well defined by the electron density with a few exceptions: The N-terminal residues 296 to 330 and the C-terminal residues 604 to 625 are completely disordered and therefore not visible in the x-ray structure. There are a few side chains at the surface of the molecules that do not show a well-defined electron density. A number of side chains clearly show alternating side chain positions. Those were not refined; there is only one side chain with alternating conformation close to the staurosporin-binding site, which could be of importance: SER 478.

There is an electron density of the linker region between β5 and αD. This region has an unusual sequence (Ala417 - Gly418 - Gly419 - Gly420 - Pro421) and forms part of the staurosporine binding site. This region is well ordered and the electron density is well defined. The two important contacts (Glu 415O - N1, Ala 417N - O5).

Staurosporine-binding site

The binding site for staurosporine in mostly shaped by the hydrophobic side chains of the following residues: Leu344, Phe349, Val352, Val399, Met414, Met416, Ala417, Leu468. Deep in the binding pocket, two polar interactions contribute to the staurosporine binding: the main chain carbonyl oxygen of residue Glu415 binds to nitrogen N1 of staurosporine and the main chain peptide nitrogen of residue Ala417 interacts with the carbonyl oxygen O5 of staurosporine. At the other end of the staurosporine molecule there are a few polar interactions between the sugar moiety and the protein. The staurosporine methoxy group

forms only van der Waals contacts, but the -N-Met group interacts with the protein through a hydrogen bridge network that is formed by a number of solvent molecules and the side chains of residue Lys424, His423, Arg465 (also involving the carboxyl oxygen of the peptide bond), Asp479, Asn466.

An alignment (ClustalW) with some of the well-known kinase structures show that the sequence variability is rather high. Nevertheless, if the c-alpha traces get superimposed, usually a relatively good fit is noticed (53-59%).

From the alignment, many kinases have insertions or deletions compared to Zap70 which makes is extremely difficult to model the structure in every detail. Nevertheless, the ATP-binding site has a relatively conserved structure and is easier to model than most of the rest of the kinase domain.

Phosphorylation sites

Phosphorylation of residues in the activation segment causes conformational changes in the catalytic kinase domain that lead to the correct positioning of substrate binding residues and catalytic residues, and relief of steric blocking to enable access of substrate to the catalytic site.

The kinase domain crystallized here, is not phosphorylated. However, Zap70 contains a number of tyrosine residues, which can be phosphorylated in vivo and contribute to the regulation of the kinase activity and adaptor molecule binding. Due to the fact, that we are targeting the ATP binding site, it should not be a huge drawback that we only have the structure of the non-activated/phosphorylated kinase domain.

The phosphorylation sites 474, 492, 493, 597, and 598 are defined in the x-ray structure. Tyrosine 492 and 493 are both located in the activation loop. Transphosphorylation of Tyrosine 493 by Lck leads to activation of Zap70. (Chan, et al 1995, Wange et al 1995, Mège, et al 1996) This tyrosine residue corresponds to Tyrosine 1163 of the insulin receptor kinase domain which causes upon transphosphorylation, a major conformational change of the activation loop (Hubbard 1997). It is thus likely that the structure of the corresponding activation loop of ZAP-70 phosphorylated at Tyrosine 493 will be different than the one shown here. The role of Tyrosine 492 is less clear. A negative regulatory function has been

proposed (Chan, et al 1995). Tyrosine 474 is required for association with the Shc adapter, which couples T cell receptor signaling to the Ras pathway (Pacini, et al 1998). The surface exposed Tyrosine 474 is located at the beginning of the β8 segment, close to the following activation segment. Tyrosine 597 and 598 located at the surface of the protein near to the C-terminus are supposed to be involved in regulating the functional activity of ZAP-70 possibly by inhibitory proteins (Zeitlmann, et al 1998).

atomic coordinates.txt
Table 1: Atomic Coordinates of ZAP-70 Catalytic Domain with Staurosporine

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REMARK   3   PROGRAM        : CNX 2000.1
REMARK   3   AUTHORS        : Brunger, Adams, Clore, Delano,
REMARK   3                    Gros, Grosse-Kunstleve, Jiang,
REMARK   3                    Kuszewski, Nilges, Pannu, Read,
REMARK   3                    Rice, Simonson, Warren
REMARK   3                    and
REMARK   3                    Molecular Simulations Inc.,
REMARK   3                    (Badger, Berard, Kumar, Szalma,
REMARK   3                    Yip).
REMARK   3
REMARK   3   DATA USED IN REFINEMENT.
REMARK   3    RESOLUTION RANGE HIGH (ANGSTROMS) : 1.90
REMARK   3    RESOLUTION RANGE LOW  (ANGSTROMS) :  19.26
REMARK   3    DATA CUTOFF            (SIGMA(F)) : 0.0
REMARK   3    DATA CUTOFF HIGH        (ABS(F)) :   933984.58
REMARK   3    DATA CUTOFF LOW         (ABS(F)) :     0.000000
REMARK   3    COMPLETENESS (WORKING+TEST)   (%) : 96.7
REMARK   3    NUMBER OF REFLECTIONS             : 45463
REMARK   3
REMARK   3   FIT TO DATA USED IN REFINEMENT.
REMARK   3    CROSS-VALIDATION METHOD          : THROUGHOUT
REMARK   3    FREE R VALUE TEST SET SELECTION  : RANDOM
REMARK   3    R VALUE            (WORKING SET) : 0.182
REMARK   3    FREE R VALUE                     : 0.209
REMARK   3    FREE R VALUE TEST SET SIZE   (%) : 5.0
REMARK   3    FREE R VALUE TEST SET COUNT      : 2284
REMARK   3    ESTIMATED ERROR OF FREE R VALUE  : 0.004
REMARK   3
REMARK   3   FIT IN THE HIGHEST RESOLUTION BIN.
REMARK   3    TOTAL NUMBER OF BINS USED          :     6
REMARK   3    BIN RESOLUTION RANGE HIGH      (A) : 1.90
REMARK   3    BIN RESOLUTION RANGE LOW       (A) : 2.02
REMARK   3    BIN COMPLETENESS (WORKING+TEST) (%) : 93.7
REMARK   3    REFLECTIONS IN BIN    (WORKING SET) :  6918
REMARK   3    BIN R VALUE           (WORKING SET) : 0.195
REMARK   3    BIN FREE R VALUE                    : 0.241
REMARK   3    BIN FREE R VALUE TEST SET SIZE  (%) : 5.2
REMARK   3    BIN FREE R VALUE TEST SET COUNT     :   378
REMARK   3    ESTIMATED ERROR OF BIN FREE R VALUE : 0.012
REMARK   3
REMARK   3   NUMBER OF NON-HYDROGEN ATOMS USED IN REFINEMENT.
REMARK   3    PROTEIN ATOMS             : 4739
REMARK   3    NUCLEIC ACID ATOMS        :    0
REMARK   3    HETEROGEN ATOMS           :    0
REMARK   3    SOLVENT ATOMS             :    0
REMARK   3
REMARK   3   B VALUES.
REMARK   3    FROM WILSON PLOT          (A**2) : 24.1
REMARK   3    MEAN B VALUE     (OVERALL, A**2) : 35.0
REMARK   3    OVERALL ANISOTROPIC B VALUE.
REMARK   3     B11 (A**2) :  0.16
REMARK   3     B22 (A**2) : -1.31
REMARK   3     B33 (A**2) :  1.15
REMARK   3     B12 (A**2) :  0.00
REMARK   3     B13 (A**2) :  2.08
REMARK   3     B23 (A**2) : -1.25
REMARK   3
REMARK   3   BULK SOLVENT MODELING.
REMARK   3    METHOD USED : FLAT MODEL
REMARK   3    KSOL        : 0.38494
REMARK   3    BSOL        : 52.9849 (A**2)
REMARK   3
REMARK   3   ESTIMATED COORDINATE ERROR.
REMARK   3    ESD FROM LUZZATI PLOT      (A) : 0.19
REMARK   3    ESD FROM SIGMAA            (A) : 0.01
REMARK   3    LOW RESOLUTION CUTOFF      (A) : 5.00
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                        atomic coordinates.txt
REMARK   3
REMARK   3
REMARK   3  CROSS-VALIDATED ESTIMATED COORDINATE ERROR.
REMARK   3   ESD FROM C-V LUZZATI PLOT      (A) : 0.22
REMARK   3   ESD FROM C-V SIGMAA            (A) : 0.11
REMARK   3
REMARK   3  RMS DEVIATIONS FROM IDEAL VALUES.
REMARK   3   BOND LENGTHS                   (A) : 0.011
REMARK   3   BOND ANGLES               (DEGREES) : 1.3
REMARK   3   DIHEDRAL ANGLES           (DEGREES) : 21.4
REMARK   3   IMPROPER ANGLES           (DEGREES) : 0.91
REMARK   3
REMARK   3  ISOTROPIC THERMAL MODEL : RESTRAINED
REMARK   3
REMARK   3  ISOTROPIC THERMAL FACTOR RESTRAINTS.    RMS     SIGMA
REMARK   3   MAIN-CHAIN BOND              (A**2) : 3.56 ;  1.50
REMARK   3   MAIN-CHAIN ANGLE             (A**2) : 4.55 ;  2.00
REMARK   3   SIDE-CHAIN BOND              (A**2) : 4.82 ;  2.00
REMARK   3   SIDE-CHAIN ANGLE             (A**2) : 6.37 ;  2.50
REMARK   3
REMARK   3  NCS MODEL : NONE
REMARK   3
REMARK   3  NCS RESTRAINTS.                         RMS     SIGMA/WEIGHT
REMARK   3   GROUP  1  POSITIONAL          (A) : NULL  ; NULL
REMARK   3   GROUP  1  B-FACTOR         (A**2) : NULL  ; NULL
REMARK   3
REMARK   3  PARAMETER FILE  1  : MSI_CNX_TOPPAR/protein_rep.param
REMARK   3  PARAMETER FILE  2  : MSI_CNX_TOPPAR/water_rep.param
REMARK   3  PARAMETER FILE  3  : stu.param
REMARK   3  TOPOLOGY FILE   1  : MSI_CNX_TOPPAR/protein.top
REMARK   3  TOPOLOGY FILE   2  : MSI_CNX_TOPPAR/water.top
REMARK   3  TOPOLOGY FILE   3  : stu.toppar
REMARK   3
REMARK   3  OTHER REFINEMENT REMARKS: NULL
SEQRES   1 A  273  PHE LEU LYS ARG ASP ASN LEU LEU ILE ALA ASP ILE GLU
SEQRES   2 A  273  LEU GLY CYS GLY ASN PHE GLY SER VAL ARG GLN GLY VAL
SEQRES   3 A  273  TYR ARG MET ARG LYS LYS GLN ILE ASP VAL ALA ILE LYS
SEQRES   4 A  273  VAL LEU LYS GLN GLY THR GLU LYS ALA ASP THR GLU GLU
SEQRES   5 A  273  MET MET ARG GLU ALA GLN ILE MET HIS GLN LEU ASP ASN
SEQRES   6 A  273  PRO TYR ILE VAL ARG LEU ILE GLY VAL CYS GLN ALA GLU
SEQRES   7 A  273  ALA LEU MET LEU VAL MET GLU MET ALA GLY GLY GLY PRO
SEQRES   8 A  273  LEU HIS LYS PHE LEU VAL GLY LYS ARG GLU GLU ILE PRO
SEQRES   9 A  273  VAL SER ASN VAL ALA GLU LEU LEU HIS GLN VAL SER MET
SEQRES  10 A  273  GLY MET LYS TYR LEU GLU GLU LYS ASN PHE VAL HIS ARG
SEQRES  11 A  273  ASP LEU ALA ALA ARG ASN VAL LEU LEU VAL ASN ARG HIS
SEQRES  12 A  273  TYR ALA LYS ILE SER ASP PHE GLY LEU SER LYS ALA LEU
SEQRES  13 A  273  GLY ALA ASP ASP SER TYR TYR THR ALA ARG SER ALA GLY
SEQRES  14 A  273  LYS TRP PRO LEU LYS TRP TYR ALA PRO GLU CYS ILE ASN
SEQRES  15 A  273  PHE ARG LYS PHE SER SER ARG SER ASP VAL TRP SER TYR
SEQRES  16 A  273  GLY VAL THR MET TRP GLU ALA LEU SER TYR GLY GLN LYS
SEQRES  17 A  273  PRO TYR LYS LYS MET LYS GLY PRO GLU VAL MET ALA PHE
SEQRES  18 A  273  ILE GLU GLN GLY LYS ARG MET GLU CYS PRO PRO GLU CYS
SEQRES  19 A  273  PRO PRO GLU LEU TYR ALA LEU MET SER ASP CYS TRP ILE
SEQRES  20 A  273  TYR LYS TRP GLU ASP ARG PRO ASP PHE LEU THR VAL GLU
SEQRES  21 A  273  GLN ARG MET ARG ALA CYS TYR TYR SER LEU ALA SER LYS
SEQRES   1 B  273  PHE LEU LYS ARG ASP ASN LEU LEU ILE ALA ASP ILE GLU
SEQRES   2 B  273  LEU GLY CYS GLY ASN PHE GLY SER VAL ARG GLN GLY VAL
SEQRES   3 B  273  TYR ARG MET ARG LYS LYS GLN ILE ASP VAL ALA ILE LYS
SEQRES   4 B  273  VAL LEU LYS GLN GLY THR GLU LYS ALA ASP THR GLU GLU
SEQRES   5 B  273  MET MET ARG GLU ALA GLN ILE MET HIS GLN LEU ASP ASN
SEQRES   6 B  273  PRO TYR ILE VAL ARG LEU ILE GLY VAL CYS GLN ALA GLU
SEQRES   7 B  273  ALA LEU MET LEU VAL MET GLU MET ALA GLY GLY GLY PRO
SEQRES   8 B  273  LEU HIS LYS PHE LEU VAL GLY LYS ARG GLU GLU ILE PRO
SEQRES   9 B  273  VAL SER ASN VAL ALA GLU LEU LEU HIS GLN VAL SER MET
SEQRES  10 B  273  GLY MET LYS TYR LEU GLU GLU LYS ASN PHE VAL HIS ARG
SEQRES  11 B  273  ASP LEU ALA ALA ARG ASN VAL LEU LEU VAL ASN ARG HIS
SEQRES  12 B  273  TYR ALA LYS ILE SER ASP PHE GLY LEU SER LYS ALA LEU
SEQRES  13 B  273  GLY ALA ASP ASP SER TYR TYR THR ALA ARG SER ALA GLY
SEQRES  14 B  273  LYS TRP PRO LEU LYS TRP TYR ALA PRO GLU CYS ILE ASN
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                              atomic coordinates.txt
SEQRES  15 B  273  PHE ARG LYS PHE SER SER ARG SER ASP VAL TRP SER TYR
SEQRES  16 B  273  GLY VAL THR MET TRP GLU ALA LEU SER TYR GLY GLN LYS
SEQRES  17 B  273  PRO TYR LYS LYS MET LYS GLY PRO GLU VAL MET ALA PHE
SEQRES  18 B  273  ILE GLU GLN GLY LYS ARG MET GLU CYS PRO PRO GLU CYS
SEQRES  19 B  273  PRO PRO GLU LEU TYR ALA LEU MET SER ASP CYS TRP ILE
SEQRES  20 B  273  TYR LYS TRP GLU ASP ARG PRO ASP PHE LEU THR VAL GLU
SEQRES  21 B  273  GLN ARG MET ARG ALA CYS TYR TYR SER LEU ALA SER LYS
SEQRES   1 C    1  STU
SEQRES   1 D    1  STU
SEQRES   1 S  261  TIP TIP TIP TIP TIP TIP TIP TIP TIP TIP TIP TIP TIP
SEQRES   2 S  261  TIP TIP TIP TIP TIP TIP TIP TIP TIP TIP TIP TIP TIP
SEQRES   3 S  261  TIP TIP TIP TIP TIP TIP TIP TIP TIP TIP TIP TIP TIP
SEQRES   4 S  261  TIP TIP TIP TIP TIP TIP TIP TIP TIP TIP TIP TIP TIP
SEQRES   5 S  261  TIP TIP TIP TIP TIP TIP TIP TIP TIP TIP TIP TIP TIP
SEQRES   6 S  261  TIP TIP TIP TIP TIP TIP TIP TIP TIP TIP TIP TIP TIP
SEQRES   7 S  261  TIP TIP TIP TIP TIP TIP TIP TIP TIP TIP TIP TIP TIP
SEQRES   8 S  261  TIP TIP TIP TIP TIP TIP TIP TIP TIP TIP TIP TIP TIP
SEQRES   9 S  261  TIP TIP TIP TIP TIP TIP TIP TIP TIP TIP TIP TIP TIP
SEQRES  10 S  261  TIP TIP TIP TIP TIP TIP TIP TIP TIP TIP TIP TIP TIP
SEQRES  11 S  261  TIP TIP TIP TIP TIP TIP TIP TIP TIP TIP TIP TIP TIP
SEQRES  12 S  261  TIP TIP TIP TIP TIP TIP TIP TIP TIP TIP TIP TIP TIP
SEQRES  13 S  261  TIP TIP TIP TIP TIP TIP TIP TIP TIP TIP TIP TIP TIP
SEQRES  14 S  261  TIP TIP TIP TIP TIP TIP TIP TIP TIP TIP TIP TIP TIP
SEQRES  15 S  261  TIP TIP TIP TIP TIP TIP TIP TIP TIP TIP TIP TIP TIP
SEQRES  16 S  261  TIP TIP TIP TIP TIP TIP TIP TIP TIP TIP TIP TIP TIP
SEQRES  17 S  261  TIP TIP TIP TIP TIP TIP TIP TIP TIP TIP TIP TIP TIP
SEQRES  18 S  261  TIP TIP TIP TIP TIP TIP TIP TIP TIP TIP TIP TIP TIP
SEQRES  19 S  261  TIP TIP TIP TIP TIP TIP TIP TIP TIP TIP TIP TIP TIP
SEQRES  20 S  261  TIP TIP TIP TIP TIP TIP TIP TIP TIP TIP TIP TIP TIP
SEQRES  21 S  261  TIP
CRYST1   35.768   57.562   80.211  68.97  89.83  89.95 P 1           5
ORIGX1      1.000000  0.000000  0.000000        0.00000
ORIGX2      0.000000  1.000000  0.000000        0.00000
ORIGX3      0.000000  0.000000  1.000000        0.00000
SCALE1      0.027958 -0.000024 -0.000079        0.00000
SCALE2      0.000000  0.017373 -0.006679        0.00000
SCALE3      0.000000  0.000000  0.013357        0.00000
ATOM       1  CB  PHE A 331      -0.844 -23.839 -13.860  1.00 47.80           C
ATOM       2  CG  PHE A 331      -0.845 -24.256 -12.414  1.00 49.69           C
ATOM       3  CD1 PHE A 331      -2.033 -24.319 -11.699  1.00 53.17           C
ATOM       4  CD2 PHE A 331       0.342 -24.562 -11.764  1.00 47.25           C
ATOM       5  CE1 PHE A 331      -2.041 -24.679 -10.359  1.00 48.16           C
ATOM       6  CE2 PHE A 331       0.344 -24.924 -10.421  1.00 51.80           C
ATOM       7  CZ  PHE A 331      -0.849 -24.982  -9.720  1.00 49.42           C
ATOM       8  C   PHE A 331      -0.689 -21.905 -15.439  1.00 47.08           C
ATOM       9  O   PHE A 331      -1.461 -21.795 -16.393  1.00 48.72           O
ATOM      10  N   PHE A 331      -2.670 -22.155 -13.939  1.00 46.43           N
ATOM      11  CA  PHE A 331      -1.196 -22.366 -14.074  1.00 43.11           C
ATOM      12  N   LEU A 332       0.610 -21.631 -15.514  1.00 40.15           N
ATOM      13  CA  LEU A 332       1.245 -21.166 -16.746  1.00 42.89           C
ATOM      14  CB  LEU A 332       1.949 -19.824 -16.490  1.00 42.08           C
ATOM      15  CG  LEU A 332       1.135 -18.662 -15.894  1.00 41.32           C
ATOM      16  CD1 LEU A 332       2.088 -17.561 -15.415  1.00 36.46           C
ATOM      17  CD2 LEU A 332       0.146 -18.116 -16.931  1.00 40.99           C
ATOM      18  C   LEU A 332       2.273 -22.195 -17.207  1.00 41.99           C
ATOM      19  O   LEU A 332       2.746 -23.003 -16.416  1.00 41.81           O
ATOM      20  N   LYS A 333       2.615 -22.171 -18.492  1.00 42.98           N
ATOM      21  CA  LYS A 333       3.614 -23.091 -19.018  1.00 44.97           C
ATOM      22  CB  LYS A 333       3.495 -23.221 -20.537  1.00 45.64           C
ATOM      23  CG  LYS A 333       2.201 -23.857 -20.971  1.00 51.28           C
ATOM      24  CD  LYS A 333       2.310 -24.340 -22.408  1.00 57.41           C
ATOM      25  CE  LYS A 333       1.041 -25.067 -22.838  1.00 58.44           C
ATOM      26  NZ  LYS A 333       1.189 -25.656 -24.206  1.00 62.81           N
ATOM      27  C   LYS A 333       4.998 -22.577 -18.673  1.00 43.59           C
ATOM      28  O   LYS A 333       5.321 -21.420 -18.952  1.00 39.19           O
ATOM      29  N   ARG A 334       5.813 -23.455 -18.097  1.00 37.84           N
ATOM      30  CA  ARG A 334       7.167 -23.109 -17.698  1.00 42.87           C
ATOM      31  CB  ARG A 334       7.831 -24.309 -17.015  1.00 46.05           C
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atomic_coordinates.txt

ATOM	32	CG	ARG	A	334	9.264	-24.063	-16.553	1.00	41.63	C
ATOM	33	CD	ARG	A	334	9.303	-23.119	-15.368	1.00	37.46	C
ATOM	34	NE	ARG	A	334	10.669	-22.817	-14.947	1.00	37.67	N
ATOM	35	CZ	ARG	A	334	11.471	-21.972	-15.580	1.00	41.87	C
ATOM	36	NH1	ARG	A	334	11.038	-21.340	-16.671	1.00	38.44	N
ATOM	37	NH2	ARG	A	334	12.699	-21.747	-15.121	1.00	41.45	N
ATOM	38	C	ARG	A	334	7.999	-22.691	-18.905	1.00	42.10	C
ATOM	39	O	ARG	A	334	8.981	-21.961	-18.769	1.00	39.41	O
ATOM	40	N	ASP	A	335	7.587	-23.169	-20.077	1.00	43.76	N
ATOM	41	CA	ASP	A	335	8.274	-22.895	-21.340	1.00	44.45	C
ATOM	42	CB	ASP	A	335	7.718	-23.822	-22.423	1.00	52.46	C
ATOM	43	CG	ASP	A	335	7.632	-25.261	-21.962	1.00	55.02	C
ATOM	44	OD1	ASP	A	335	8.688	-25.925	-21.897	1.00	60.98	O
ATOM	45	OD2	ASP	A	335	6.512	-25.723	-21.643	1.00	62.85	O
ATOM	46	C	ASP	A	335	8.110	-21.455	-21.789	1.00	43.50	C
ATOM	47	O	ASP	A	335	8.904	-20.951	-22.594	1.00	41.39	O
ATOM	48	N	ASN	A	336	7.079	-20.783	-21.287	1.00	30.71	N
ATOM	49	CA	ASN	A	336	6.837	-19.407	-21.673	1.00	33.27	C
ATOM	50	CB	ASN	A	336	5.341	-19.129	-21.723	1.00	36.84	C
ATOM	51	CG	ASN	A	336	4.647	-19.915	-22.809	1.00	49.26	C
ATOM	52	OD1	ASN	A	336	5.193	-20.109	-23.899	1.00	49.53	O
ATOM	53	ND2	ASN	A	336	3.426	-20.351	-22.527	1.00	48.43	N
ATOM	54	C	ASN	A	336	7.494	-18.421	-20.731	1.00	28.53	C
ATOM	55	O	ASN	A	336	7.363	-17.210	-20.895	1.00	30.15	O
ATOM	56	N	LEU	A	337	8.203	-18.948	-19.749	1.00	32.36	N
ATOM	57	CA	LEU	A	337	8.855	-18.115	-18.750	1.00	34.27	C
ATOM	58	CB	LEU	A	337	8.365	-18.518	-17.350	1.00	30.14	C
ATOM	59	CG	LEU	A	337	8.920	-17.781	-16.125	1.00	28.85	C
ATOM	60	CD1	LEU	A	337	8.290	-16.416	-16.039	1.00	27.73	C
ATOM	61	CD2	LEU	A	337	8.586	-18.559	-14.850	1.00	35.78	C
ATOM	62	C	LEU	A	337	10.380	-18.202	-18.800	1.00	31.60	C
ATOM	63	O	LEU	A	337	10.956	-19.279	-18.875	1.00	32.32	O
ATOM	64	N	LEU	A	338	11.032	-17.051	-18.741	1.00	25.65	N
ATOM	65	CA	LEU	A	338	12.486	-17.006	-18.731	1.00	24.94	C
ATOM	66	CB	LEU	A	338	13.020	-16.257	-19.977	1.00	28.20	C
ATOM	67	CG	LEU	A	338	14.554	-16.272	-20.089	1.00	30.23	C
ATOM	68	CD1	LEU	A	338	15.028	-17.702	-20.306	1.00	33.75	C
ATOM	69	CD2	LEU	A	338	15.012	-15.400	-21.245	1.00	31.10	C
ATOM	70	C	LEU	A	338	12.855	-16.235	-17.465	1.00	29.76	C
ATOM	71	O	LEU	A	338	12.624	-15.030	-17.384	1.00	30.99	O
ATOM	72	N	ILE	A	339	13.401	-16.933	-16.471	1.00	30.96	N
ATOM	73	CA	ILE	A	339	13.763	-16.266	-15.219	1.00	29.19	C
ATOM	74	CB	ILE	A	339	13.645	-17.230	-14.011	1.00	33.77	C
ATOM	75	CG2	ILE	A	339	13.912	-16.458	-12.704	1.00	30.52	C
ATOM	76	CG1	ILE	A	339	12.267	-17.901	-14.025	1.00	32.27	C
ATOM	77	CD1	ILE	A	339	12.057	-18.955	-12.960	1.00	38.69	C
ATOM	78	C	ILE	A	339	15.185	-15.743	-15.277	1.00	31.14	C
ATOM	79	O	ILE	A	339	16.119	-16.500	-15.534	1.00	34.19	O
ATOM	80	N	ALA	A	340	15.347	-14.448	-15.029	1.00	29.75	N
ATOM	81	CA	ALA	A	340	16.676	-13.843	-15.055	1.00	34.31	C
ATOM	82	CB	ALA	A	340	16.569	-12.342	-15.334	1.00	32.66	C
ATOM	83	C	ALA	A	340	17.406	-14.090	-13.736	1.00	36.59	C
ATOM	84	O	ALA	A	340	16.788	-14.463	-12.724	1.00	34.25	O
ATOM	85	N	ASP	A	341	18.718	-13.901	-13.745	1.00	33.86	N
ATOM	86	CA	ASP	A	341	19.514	-14.093	-12.542	1.00	37.73	C
ATOM	87	CB	ASP	A	341	20.924	-14.582	-12.911	1.00	45.65	C
ATOM	88	CG	ASP	A	341	21.639	-15.259	-11.738	1.00	56.30	C
ATOM	89	OD1	ASP	A	341	21.455	-14.811	-10.588	1.00	59.09	O
ATOM	90	OD2	ASP	A	341	22.399	-16.234	-11.966	1.00	62.33	O
ATOM	91	C	ASP	A	341	19.594	-12.739	-11.850	1.00	43.58	C
ATOM	92	O	ASP	A	341	20.683	-12.245	-11.562	1.00	44.94	O
ATOM	93	N	ILE	A	342	18.434	-12.134	-11.595	1.00	36.82	N
ATOM	94	CA	ILE	A	342	18.349	-10.829	-10.954	1.00	35.58	C
ATOM	95	CB	ILE	A	342	17.894	-9.763	-11.969	1.00	38.49	C
ATOM	96	CG2	ILE	A	342	17.708	-8.407	-11.281	1.00	43.25	C
ATOM	97	CG1	ILE	A	342	18.912	-9.675	-13.106	1.00	36.31	C
ATOM	98	CD1	ILE	A	342	18.468	-8.769	-14.239	1.00	46.83	C
ATOM	99	C	ILE	A	342	17.327	-10.911	-9.825	1.00	37.22	C

atomic_coordinates.txt

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ATOM   100   O    ILE A 342     16.214 -11.364 -10.037  1.00 31.02         O
ATOM   101   N    GLU A 343     17.710 -10.475  -8.633  1.00 33.59         N
ATOM   102   CA   GLU A 343     16.816 -10.526  -7.485  1.00 36.18         C
ATOM   103   CB   GLU A 343     17.566 -11.064  -6.264  1.00 36.52         C
ATOM   104   CG   GLU A 343     16.713 -11.123  -5.003  1.00 40.70         C
ATOM   105   CD   GLU A 343     17.356 -11.929  -3.889  1.00 48.49         C
ATOM   106   OE1  GLU A 343     17.391 -13.175  -3.992  1.00 50.24         O
ATOM   107   OE2  GLU A 343     17.833 -11.314  -2.915  1.00 51.47         O
ATOM   108   C    GLU A 343     16.263  -9.143  -7.180  1.00 37.22         C
ATOM   109   O    GLU A 343     17.031  -8.236  -6.890  1.00 32.38         O
ATOM   110   N    LEU A 344     14.937  -8.989  -7.246  1.00 25.47         N
ATOM   111   CA   LEU A 344     14.317  -7.693  -6.969  1.00 23.40         C
ATOM   112   CB   LEU A 344     12.916  -7.594  -7.644  1.00 23.43         C
ATOM   113   CG   LEU A 344     12.969  -7.779  -9.161  1.00 32.75         C
ATOM   114   CD1  LEU A 344     11.538  -7.940  -9.704  1.00 27.03         C
ATOM   115   CD2  LEU A 344     13.684  -6.585  -9.819  1.00 32.92         C
ATOM   116   C    LEU A 344     14.185  -7.494  -5.471  1.00 25.30         C
ATOM   117   O    LEU A 344     14.236  -6.365  -4.982  1.00 29.77         O
ATOM   118   N    GLY A 345     13.997  -8.591  -4.736  1.00 25.68         N
ATOM   119   CA   GLY A 345     13.884  -8.500  -3.296  1.00 27.74         C
ATOM   120   C    GLY A 345     13.777  -9.886  -2.700  1.00 29.98         C
ATOM   121   O    GLY A 345     13.835 -10.872  -3.418  1.00 31.85         O
ATOM   122   N    CYS A 346     13.638  -9.976  -1.382  1.00 29.57         N
ATOM   123   CA   CYS A 346     13.498 -11.286  -0.755  1.00 32.14         C
ATOM   124   CB   CYS A 346     14.867 -11.885  -0.465  1.00 38.98         C
ATOM   125   SG   CYS A 346     15.741 -10.909   0.749  1.00 43.33         S
ATOM   126   C    CYS A 346     12.719 -11.167   0.544  1.00 36.85         C
ATOM   127   O    CYS A 346     12.395 -10.063   0.978  1.00 38.86         O
ATOM   128   N    GLY A 347     12.428 -12.316   1.142  1.00 36.28         N
ATOM   129   CA   GLY A 347     11.704 -12.369   2.402  1.00 35.52         C
ATOM   130   C    GLY A 347     11.923 -13.746   2.997  1.00 35.81         C
ATOM   131   O    GLY A 347     12.671 -14.541   2.435  1.00 32.94         O
ATOM   132   N    ASN A 348     11.272 -14.040   4.116  1.00 39.18         N
ATOM   133   CA   ASN A 348     11.406 -15.350   4.749  1.00 42.21         C
ATOM   134   CB   ASN A 348     10.644 -15.387   6.080  1.00 48.61         C
ATOM   135   CG   ASN A 348     11.277 -14.514   7.131  1.00 53.37         C
ATOM   136   OD1  ASN A 348     12.442 -14.702   7.492  1.00 56.08         O
ATOM   137   ND2  ASN A 348     10.516 -13.546   7.635  1.00 59.19         N
ATOM   138   C    ASN A 348     10.881 -16.464   3.852  1.00 39.31         C
ATOM   139   O    ASN A 348     11.275 -17.619   3.996  1.00 39.22         O
ATOM   140   N    PHE A 349      9.980 -16.116   2.933  1.00 35.86         N
ATOM   141   CA   PHE A 349      9.404 -17.095   2.016  1.00 32.64         C
ATOM   142   CB   PHE A 349      8.143 -16.518   1.352  1.00 37.33         C
ATOM   143   CG   PHE A 349      8.416 -15.318   0.467  1.00 33.86         C
ATOM   144   CD1  PHE A 349      9.019 -15.475  -0.777  1.00 38.44         C
ATOM   145   CD2  PHE A 349      8.121 -14.031   0.905  1.00 37.11         C
ATOM   146   CE1  PHE A 349      9.332 -14.360  -1.573  1.00 37.32         C
ATOM   147   CE2  PHE A 349      8.427 -12.917   0.123  1.00 38.27         C
ATOM   148   CZ   PHE A 349      9.036 -13.082  -1.120  1.00 36.15         C
ATOM   149   C    PHE A 349     10.394 -17.491   0.919  1.00 33.34         C
ATOM   150   O    PHE A 349     10.333 -18.586   0.367  1.00 36.04         O
ATOM   151   N    GLY A 350     11.287 -16.575   0.574  1.00 36.72         N
ATOM   152   CA   GLY A 350     12.234 -16.848  -0.490  1.00 29.36         C
ATOM   153   C    GLY A 350     12.627 -15.562  -1.166  1.00 32.07         C
ATOM   154   O    GLY A 350     12.959 -14.591  -0.506  1.00 37.38         O
ATOM   155   N    SER A 351     12.595 -15.526  -2.493  1.00 34.36         N
ATOM   156   CA   SER A 351     12.993 -14.304  -3.151  1.00 33.56         C
ATOM   157   CB   SER A 351     14.439 -14.414  -3.605  1.00 39.89         C
ATOM   158   OG   SER A 351     14.564 -15.336  -4.654  1.00 38.83         O
ATOM   159   C    SER A 351     12.093 -13.929  -4.318  1.00 25.34         C
ATOM   160   O    SER A 351     11.246 -14.703  -4.741  1.00 30.57         O
ATOM   161   N    VAL A 352     12.282 -12.719  -4.812  1.00 25.32         N
ATOM   162   CA   VAL A 352     11.484 -12.243  -5.934  1.00 27.67         C
ATOM   163   CB   VAL A 352     10.777 -10.928  -5.596  1.00 26.27         C
ATOM   164   CG1  VAL A 352      9.988 -10.443  -6.807  1.00 28.62         C
ATOM   165   CG2  VAL A 352      9.846 -11.136  -4.387  1.00 25.93         C
ATOM   166   C    VAL A 352     12.504 -12.002  -7.022  1.00 24.75         C
ATOM   167   O    VAL A 352     13.416 -11.177  -6.862  1.00 26.64         O
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ATOM	168	N	ARG	A	353	12.334	-12.720	-8.124	1.00 21.24	N
ATOM	169	CA	ARG	A	353	13.259	-12.640	-9.253	1.00 24.10	C
ATOM	170	CB	ARG	A	353	13.643	-14.052	-9.721	1.00 24.70	C
ATOM	171	CG	ARG	A	353	14.430	-14.913	-8.722	1.00 41.94	C
ATOM	172	CD	ARG	A	353	15.851	-14.401	-8.516	1.00 48.67	C
ATOM	173	NE	ARG	A	353	16.805	-15.494	-8.339	1.00 56.82	N
ATOM	174	CZ	ARG	A	353	17.287	-16.243	-9.330	1.00 59.51	C
ATOM	175	NH1	ARG	A	353	16.913	-16.024	-10.585	1.00 54.48	N
ATOM	176	NH2	ARG	A	353	18.140	-17.226	-9.065	1.00 58.82	N
ATOM	177	C	ARG	A	353	12.625	-11.910	-10.430	1.00 30.05	C
ATOM	178	O	ARG	A	353	11.403	-11.914	-10.605	1.00 32.28	O
ATOM	179	N	GLN	A	354	13.461	-11.288	-11.245	1.00 26.89	N
ATOM	180	CA	GLN	A	354	12.954	-10.605	-12.429	1.00 21.13	C
ATOM	181	CB	GLN	A	354	13.886	-9.449	-12.813	1.00 27.45	C
ATOM	182	CG	GLN	A	354	13.394	-8.651	-14.005	1.00 33.20	C
ATOM	183	CD	GLN	A	354	14.196	-7.386	-14.228	1.00 35.81	C
ATOM	184	OE1	GLN	A	354	14.929	-6.932	-13.344	1.00 32.36	O
ATOM	185	NE2	GLN	A	354	14.048	-6.798	-15.410	1.00 38.36	N
ATOM	186	C	GLN	A	354	12.954	-11.650	-13.537	1.00 26.03	C
ATOM	187	O	GLN	A	354	13.773	-12.580	-13.516	1.00 27.62	O
ATOM	188	N	GLY	A	355	12.044	-11.498	-14.498	1.00 23.59	N
ATOM	189	CA	GLY	A	355	12.005	-12.421	-15.612	1.00 23.56	C
ATOM	190	C	GLY	A	355	11.167	-11.834	-16.740	1.00 28.28	C
ATOM	191	O	GLY	A	355	10.786	-10.665	-16.702	1.00 25.55	O
ATOM	192	N	VAL	A	356	10.901	-12.664	-17.755	1.00 28.64	N
ATOM	193	CA	VAL	A	356	10.074	-12.264	-18.883	1.00 29.66	C
ATOM	194	CB	VAL	A	356	10.921	-12.045	-20.174	1.00 34.30	C
ATOM	195	CG1	VAL	A	356	10.005	-11.659	-21.351	1.00 32.44	C
ATOM	196	CG2	VAL	A	356	11.931	-10.977	-19.919	1.00 29.39	C
ATOM	197	C	VAL	A	356	9.108	-13.402	-19.127	1.00 23.76	C
ATOM	198	O	VAL	A	356	9.485	-14.569	-19.033	1.00 26.47	O
ATOM	199	N	TYR	A	357	7.859	-13.064	-19.438	1.00 28.83	N
ATOM	200	CA	TYR	A	357	6.847	-14.082	-19.703	1.00 29.55	C
ATOM	201	CB	TYR	A	357	5.697	-14.003	-18.693	1.00 32.75	C
ATOM	202	CG	TYR	A	357	4.603	-14.999	-18.981	1.00 31.78	C
ATOM	203	CD1	TYR	A	357	4.766	-16.355	-18.702	1.00 33.06	C
ATOM	204	CE1	TYR	A	357	3.761	-17.287	-19.010	1.00 38.12	C
ATOM	205	CD2	TYR	A	357	3.417	-14.587	-19.575	1.00 38.71	C
ATOM	206	CE2	TYR	A	357	2.410	-15.504	-19.887	1.00 39.65	C
ATOM	207	CZ	TYR	A	357	2.587	-16.844	-19.601	1.00 39.40	C
ATOM	208	OH	TYR	A	357	1.577	-17.722	-19.904	1.00 48.05	O
ATOM	209	C	TYR	A	357	6.291	-13.846	-21.098	1.00 33.01	C
ATOM	210	O	TYR	A	357	6.038	-12.699	-21.484	1.00 34.42	O
ATOM	211	N	ARG	A	358	6.093	-14.925	-21.845	1.00 40.49	N
ATOM	212	CA	ARG	A	358	5.582	-14.797	-23.201	1.00 43.14	C
ATOM	213	CB	ARG	A	358	6.303	-15.787	-24.128	1.00 42.64	C
ATOM	214	CG	ARG	A	358	5.804	-15.762	-25.580	1.00 47.94	C
ATOM	215	CD	ARG	A	358	6.599	-16.738	-26.435	1.00 46.49	C
ATOM	216	NE	ARG	A	358	6.555	-18.096	-25.898	1.00 48.83	N
ATOM	217	CZ	ARG	A	358	7.470	-19.024	-26.159	1.00 47.27	C
ATOM	218	NH1	ARG	A	358	8.496	-18.736	-26.947	1.00 48.46	N
ATOM	219	NH2	ARG	A	358	7.365	-20.239	-25.636	1.00 49.08	N
ATOM	220	C	ARG	A	358	4.083	-15.023	-23.299	1.00 37.81	C
ATOM	221	O	ARG	A	358	3.602	-16.102	-22.983	1.00 39.13	O
ATOM	222	N	MET	A	359	3.361	-13.984	-23.712	1.00 48.72	N
ATOM	223	CA	MET	A	359	1.917	-14.072	-23.926	1.00 52.67	C
ATOM	224	CB	MET	A	359	1.185	-12.898	-23.284	1.00 56.85	C
ATOM	225	CG	MET	A	359	1.487	-12.704	-21.817	1.00 59.91	C
ATOM	226	SD	MET	A	359	0.442	-11.450	-21.068	1.00 68.40	S
ATOM	227	CE	MET	A	359	1.094	-9.949	-21.845	1.00 66.35	C
ATOM	228	C	MET	A	359	1.810	-13.963	-25.443	1.00 57.95	C
ATOM	229	O	MET	A	359	2.127	-12.913	-26.006	1.00 66.19	O
ATOM	230	N	ARG	A	360	1.393	-15.043	-26.097	1.00 60.89	N
ATOM	231	CA	ARG	A	360	1.282	-15.079	-27.561	1.00 63.37	C
ATOM	232	CB	ARG	A	360	0.383	-16.246	-27.994	1.00 64.54	C
ATOM	233	CG	ARG	A	360	0.960	-17.616	-27.623	1.00 65.69	C
ATOM	234	CD	ARG	A	360	2.353	-17.786	-28.231	1.00 65.62	C
ATOM	235	NE	ARG	A	360	3.255	-18.567	-27.384	1.00 65.60	N

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ATOM   236  CZ   ARG A 360      3.082 -19.851 -27.070  1.00 63.16           C
ATOM   237  NH1  ARG A 360      2.027 -20.525 -27.527  1.00 62.71           N
ATOM   238  NH2  ARG A 360      3.977 -20.470 -26.309  1.00 62.89           N
ATOM   239  C    ARG A 360      0.788 -13.774 -28.175  1.00 63.27           C
ATOM   240  O    ARG A 360     -0.417 -13.601 -28.401  1.00 68.94           O
ATOM   241  N    LYS A 361      1.743 -12.878 -28.448  1.00 59.53           N
ATOM   242  CA   LYS A 361      1.511 -11.549 -29.022  1.00 56.77           C
ATOM   243  CB   LYS A 361      0.219 -10.938 -28.461  1.00 60.05           C
ATOM   244  CG   LYS A 361      0.226 -10.722 -26.950  1.00 60.48           C
ATOM   245  CD   LYS A 361     -1.174 -10.402 -26.409  1.00 62.81           C
ATOM   246  CE   LYS A 361     -1.771  -9.144 -27.036  1.00 64.09           C
ATOM   247  NZ   LYS A 361     -3.154  -8.872 -26.526  1.00 65.39           N
ATOM   248  C    LYS A 361      2.701 -10.647 -28.659  1.00 61.19           C
ATOM   249  O    LYS A 361      3.151  -9.813 -29.464  1.00 60.48           O
ATOM   250  N    LYS A 362      3.204 -10.819 -27.436  1.00 52.69           N
ATOM   251  CA   LYS A 362      4.334 -10.035 -26.949  1.00 54.92           C
ATOM   252  CB   LYS A 362      3.901  -8.588 -26.737  1.00 56.85           C
ATOM   253  CG   LYS A 362      2.785  -8.432 -25.728  1.00 53.56           C
ATOM   254  CD   LYS A 362      2.334  -6.986 -25.680  1.00 58.19           C
ATOM   255  CE   LYS A 362      1.452  -6.738 -24.479  1.00 60.02           C
ATOM   256  NZ   LYS A 362      0.281  -7.656 -24.462  1.00 59.99           N
ATOM   257  C    LYS A 362      4.900 -10.601 -25.642  1.00 48.81           C
ATOM   258  O    LYS A 362      4.298 -11.460 -25.015  1.00 48.05           O
ATOM   259  N    GLN A 363      6.069 -10.119 -25.241  1.00 51.22           N
ATOM   260  CA   GLN A 363      6.682 -10.594 -24.007  1.00 49.77           C
ATOM   261  CB   GLN A 363      8.095 -11.132 -24.267  1.00 54.46           C
ATOM   262  CG   GLN A 363      8.154 -12.259 -25.286  1.00 52.95           C
ATOM   263  CD   GLN A 363      9.545 -12.865 -25.397  1.00 54.97           C
ATOM   264  OE1  GLN A 363     10.550 -12.189 -25.172  1.00 58.63           O
ATOM   265  NE2  GLN A 363      9.606 -14.135 -25.764  1.00 57.23           N
ATOM   266  C    GLN A 363      6.737  -9.459 -23.014  1.00 46.14           C
ATOM   267  O    GLN A 363      7.198  -8.366 -23.329  1.00 52.39           O
ATOM   268  N    ILE A 364      6.269  -9.716 -21.799  1.00 38.56           N
ATOM   269  CA   ILE A 364      6.266  -8.671 -20.796  1.00 38.92           C
ATOM   270  CB   ILE A 364      4.865  -8.450 -20.233  1.00 46.04           C
ATOM   271  CG2  ILE A 364      3.907  -8.072 -21.353  1.00 42.34           C
ATOM   272  CG1  ILE A 364      4.388  -9.715 -19.542  1.00 38.48           C
ATOM   273  CD1  ILE A 364      3.262  -9.453 -18.591  1.00 46.96           C
ATOM   274  C    ILE A 364      7.199  -8.974 -19.643  1.00 35.15           C
ATOM   275  O    ILE A 364      7.473 -10.142 -19.337  1.00 29.70           O
ATOM   276  N    ASP A 365      7.685  -7.922 -19.005  1.00 32.92           N
ATOM   277  CA   ASP A 365      8.577  -8.086 -17.872  1.00 31.39           C
ATOM   278  CB   ASP A 365      9.253  -6.762 -17.552  1.00 35.51           C
ATOM   279  CG   ASP A 365     10.142  -6.278 -18.685  1.00 40.87           C
ATOM   280  OD1  ASP A 365     10.983  -7.066 -19.158  1.00 44.73           O
ATOM   281  OD2  ASP A 365      9.997  -5.102 -19.089  1.00 47.04           O
ATOM   282  C    ASP A 365      7.728  -8.520 -16.663  1.00 31.78           C
ATOM   283  O    ASP A 365      6.656  -7.977 -16.442  1.00 31.99           O
ATOM   284  N    VAL A 366      8.214  -9.484 -15.889  1.00 25.27           N
ATOM   285  CA   VAL A 366      7.472  -9.945 -14.722  1.00 24.77           C
ATOM   286  CB   VAL A 366      6.831 -11.346 -14.959  1.00 21.57           C
ATOM   287  CG1  VAL A 366      5.761 -11.282 -16.055  1.00 23.23           C
ATOM   288  CG2  VAL A 366      7.923 -12.389 -15.281  1.00 24.77           C
ATOM   289  C    VAL A 366      8.365 -10.061 -13.486  1.00 26.20           C
ATOM   290  O    VAL A 366      9.576 -10.016 -13.580  1.00 26.40           O
ATOM   291  N    ALA A 367      7.742 -10.156 -12.315  1.00 23.36           N
ATOM   292  CA   ALA A 367      8.471 -10.354 -11.074  1.00 27.38           C
ATOM   293  CB   ALA A 367      8.166  -9.227 -10.067  1.00 25.34           C
ATOM   294  C    ALA A 367      7.911 -11.716 -10.615  1.00 29.93           C
ATOM   295  O    ALA A 367      6.703 -11.961 -10.667  1.00 29.39           O
ATOM   296  N    ILE A 368      8.799 -12.603 -10.203  1.00 26.23           N
ATOM   297  CA   ILE A 368      8.418 -13.962  -9.814  1.00 26.26           C
ATOM   298  CB   ILE A 368      9.182 -15.008 -10.677  1.00 29.25           C
ATOM   299  CG2  ILE A 368      8.711 -16.425 -10.355  1.00 27.48           C
ATOM   300  CG1  ILE A 368      8.974 -14.706 -12.168  1.00 26.91           C
ATOM   301  CD1  ILE A 368     10.261 -14.543 -12.965  1.00 35.91           C
ATOM   302  C    ILE A 368      8.744 -14.257  -8.352  1.00 26.03           C
ATOM   303  O    ILE A 368      9.893 -14.229  -7.959  1.00 24.27           O
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ATOM   304  N   LYS A 369      7.720 -14.539  -7.561 1.00 25.90        N
ATOM   305  CA  LYS A 369      7.953 -14.862  -6.156 1.00 26.26        C
ATOM   306  CB  LYS A 369      6.691 -14.547  -5.344 1.00 25.23        C
ATOM   307  CG  LYS A 369      6.822 -14.795  -3.870 1.00 31.86        C
ATOM   308  CD  LYS A 369      5.509 -14.423  -3.158 1.00 34.03        C
ATOM   309  CE  LYS A 369      5.538 -14.876  -1.716 1.00 39.65        C
ATOM   310  NZ  LYS A 369      4.354 -14.402  -0.910 1.00 31.37        N
ATOM   311  C   LYS A 369      8.298 -16.361  -6.140 1.00 27.61        C
ATOM   312  O   LYS A 369      7.474 -17.219  -6.492 1.00 29.29        O
ATOM   313  N   VAL A 370      9.532 -16.674  -5.764 1.00 26.60        N
ATOM   314  CA  VAL A 370      9.990 -18.065  -5.766 1.00 28.07        C
ATOM   315  CB  VAL A 370     11.355 -18.200  -6.481 1.00 33.07        C
ATOM   316  CG1 VAL A 370     11.721 -19.667  -6.633 1.00 38.83        C
ATOM   317  CG2 VAL A 370     11.315 -17.506  -7.841 1.00 30.80        C
ATOM   318  C   VAL A 370     10.154 -18.575  -4.340 1.00 33.33        C
ATOM   319  O   VAL A 370     10.920 -18.021  -3.558 1.00 31.84        O
ATOM   320  N   LEU A 371      9.433 -19.627  -3.996 1.00 32.52        N
ATOM   321  CA  LEU A 371      9.555 -20.176  -2.653 1.00 37.90        C
ATOM   322  CB  LEU A 371      8.383 -21.111  -2.357 1.00 40.40        C
ATOM   323  CG  LEU A 371      7.003 -20.462  -2.304 1.00 38.75        C
ATOM   324  CD1 LEU A 371      5.960 -21.529  -2.018 1.00 42.86        C
ATOM   325  CD2 LEU A 371      6.987 -19.389  -1.236 1.00 40.03        C
ATOM   326  C   LEU A 371     10.877 -20.936  -2.523 1.00 41.99        C
ATOM   327  O   LEU A 371     11.250 -21.709  -3.413 1.00 37.51        O
ATOM   328  N   LYS A 372     11.571 -20.717  -1.411 1.00 40.63        N
ATOM   329  CA  LYS A 372     12.847 -21.374  -1.151 1.00 47.85        C
ATOM   330  CB  LYS A 372     13.430 -20.879   0.176 1.00 49.15        C
ATOM   331  CG  LYS A 372     12.538 -21.128   1.390 1.00 52.08        C
ATOM   332  CD  LYS A 372     13.153 -20.548   2.655 1.00 53.51        C
ATOM   333  CE  LYS A 372     12.283 -20.840   3.875 1.00 55.66        C
ATOM   334  NZ  LYS A 372     12.885 -20.313   5.137 1.00 59.56        N
ATOM   335  C   LYS A 372     12.691 -22.894  -1.121 1.00 52.35        C
ATOM   336  O   LYS A 372     11.591 -23.413  -0.941 1.00 50.37        O
ATOM   337  N   GLN A 373     13.799 -23.605  -1.312 1.00 59.78        N
ATOM   338  CA  GLN A 373     13.780 -25.067  -1.304 1.00 59.32        C
ATOM   339  CB  GLN A 373     15.115 -25.606  -1.835 1.00 63.62        C
ATOM   340  CG  GLN A 373     15.155 -27.116  -2.051 1.00 66.24        C
ATOM   341  CD  GLN A 373     14.191 -27.586  -3.134 1.00 71.01        C
ATOM   342  OE1 GLN A 373     12.970 -27.465  -2.995 1.00 69.21        O
ATOM   343  NE2 GLN A 373     14.739 -28.129  -4.219 1.00 68.75        N
ATOM   344  C   GLN A 373     13.529 -25.584   0.116 1.00 60.87        C
ATOM   345  O   GLN A 373     14.088 -25.061   1.085 1.00 58.13        O
ATOM   346  N   GLY A 374     12.673 -26.595   0.238 1.00 60.47        N
ATOM   347  CA  GLY A 374     12.378 -27.150   1.548 1.00 63.49        C
ATOM   348  C   GLY A 374     11.112 -26.589   2.169 1.00 65.45        C
ATOM   349  O   GLY A 374     10.744 -26.960   3.287 1.00 64.91        O
ATOM   350  N   THR A 375     10.448 -25.694   1.440 1.00 64.08        N
ATOM   351  CA  THR A 375      9.211 -25.073   1.910 1.00 62.35        C
ATOM   352  CB  THR A 375      8.624 -24.117   0.837 1.00 61.07        C
ATOM   353  OG1 THR A 375      9.499 -22.997   0.658 1.00 58.51        O
ATOM   354  CG2 THR A 375      7.251 -23.619   1.255 1.00 60.44        C
ATOM   355  C   THR A 375      8.164 -26.128   2.254 1.00 60.26        C
ATOM   356  O   THR A 375      7.812 -26.960   1.420 1.00 61.11        O
ATOM   357  N   GLU A 376      7.669 -26.085   3.486 1.00 61.48        N
ATOM   358  CA  GLU A 376      6.659 -27.038   3.937 1.00 63.66        C
ATOM   359  CB  GLU A 376      6.395 -26.854   5.431 1.00 65.34        C
ATOM   360  CG  GLU A 376      5.410 -27.863   6.011 1.00 70.83        C
ATOM   361  CD  GLU A 376      5.443 -27.905   7.531 1.00 74.17        C
ATOM   362  OE1 GLU A 376      5.151 -26.868   8.174 1.00 71.51        O
ATOM   363  OE2 GLU A 376      5.765 -28.983   8.083 1.00 74.47        O
ATOM   364  C   GLU A 376      5.365 -26.847   3.157 1.00 64.69        C
ATOM   365  O   GLU A 376      5.071 -25.745   2.693 1.00 62.88        O
ATOM   366  N   LYS A 377      4.595 -27.921   3.015 1.00 60.06        N
ATOM   367  CA  LYS A 377      3.339 -27.860   2.282 1.00 61.26        C
ATOM   368  CB  LYS A 377      2.637 -29.219   2.317 1.00 66.02        C
ATOM   369  CG  LYS A 377      1.309 -29.238   1.575 1.00 65.91        C
ATOM   370  CD  LYS A 377      0.916 -30.656   1.195 1.00 71.13        C
ATOM   371  CE  LYS A 377     -0.343 -30.679   0.335 1.00 69.84        C
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ATOM	372	NZ	LYS	A	377	-0.745	-32.070	-0.037	1.00	70.61	N
ATOM	373	C	LYS	A	377	2.405	-26.794	2.833	1.00	60.41	C
ATOM	374	O	LYS	A	377	1.535	-26.293	2.121	1.00	58.25	O
ATOM	375	N	ALA	A	378	2.586	-26.456	4.104	1.00	60.36	N
ATOM	376	CA	ALA	A	378	1.757	-25.450	4.756	1.00	60.42	C
ATOM	377	CB	ALA	A	378	2.126	-25.353	6.232	1.00	60.96	C
ATOM	378	C	ALA	A	378	1.914	-24.083	4.090	1.00	58.57	C
ATOM	379	O	ALA	A	378	0.928	-23.406	3.792	1.00	58.22	O
ATOM	380	N	ASP	A	379	3.159	-23.690	3.849	1.00	58.14	N
ATOM	381	CA	ASP	A	379	3.446	-22.398	3.237	1.00	59.61	C
ATOM	382	CB	ASP	A	379	4.889	-21.999	3.513	1.00	61.20	C
ATOM	383	CG	ASP	A	379	5.387	-22.533	4.841	1.00	69.25	C
ATOM	384	OD1	ASP	A	379	4.801	-22.184	5.892	1.00	70.24	O
ATOM	385	OD2	ASP	A	379	6.367	-23.313	4.831	1.00	70.38	O
ATOM	386	C	ASP	A	379	3.198	-22.428	1.730	1.00	57.10	C
ATOM	387	O	ASP	A	379	2.944	-21.394	1.118	1.00	54.39	O
ATOM	388	N	THR	A	380	3.279	-23.616	1.137	1.00	51.67	N
ATOM	389	CA	THR	A	380	3.023	-23.766	-0.287	1.00	52.52	C
ATOM	390	CB	THR	A	380	3.350	-25.193	-0.755	1.00	53.17	C
ATOM	391	OG1	THR	A	380	4.769	-25.392	-0.709	1.00	55.35	O
ATOM	392	CG2	THR	A	380	2.858	-25.411	-2.168	1.00	57.49	C
ATOM	393	C	THR	A	380	1.536	-23.488	-0.506	1.00	53.07	C
ATOM	394	O	THR	A	380	1.142	-22.808	-1.449	1.00	46.30	O
ATOM	395	N	GLU	A	381	0.714	-24.029	0.386	1.00	48.31	N
ATOM	396	CA	GLU	A	381	-0.726	-23.844	0.310	1.00	49.46	C
ATOM	397	CB	GLU	A	381	-1.421	-24.722	1.355	1.00	55.95	C
ATOM	398	CG	GLU	A	381	-2.487	-25.651	0.794	1.00	57.87	C
ATOM	399	CD	GLU	A	381	-1.909	-26.852	0.064	1.00	66.85	C
ATOM	400	OE1	GLU	A	381	-1.256	-26.663	-0.988	1.00	67.42	O
ATOM	401	OE2	GLU	A	381	-2.112	-27.992	0.547	1.00	68.23	O
ATOM	402	C	GLU	A	381	-1.025	-22.371	0.585	1.00	47.48	C
ATOM	403	O	GLU	A	381	-1.985	-21.810	0.061	1.00	44.28	O
ATOM	404	N	GLU	A	382	-0.181	-21.752	1.404	1.00	42.74	N
ATOM	405	CA	GLU	A	382	-0.332	-20.346	1.764	1.00	44.98	C
ATOM	406	CB	GLU	A	382	0.697	-19.989	2.828	1.00	50.35	C
ATOM	407	CG	GLU	A	382	0.552	-18.600	3.407	1.00	54.73	C
ATOM	408	CD	GLU	A	382	1.479	-18.376	4.593	1.00	61.59	C
ATOM	409	OE1	GLU	A	382	2.719	-18.344	4.400	1.00	67.89	O
ATOM	410	OE2	GLU	A	382	0.963	-18.241	5.726	1.00	66.58	O
ATOM	411	C	GLU	A	382	-0.150	-19.453	0.531	1.00	43.95	C
ATOM	412	O	GLU	A	382	-0.893	-18.490	0.331	1.00	37.04	O
ATOM	413	N	MET	A	383	0.847	-19.772	-0.288	1.00	38.03	N
ATOM	414	CA	MET	A	383	1.063	-18.984	-1.490	1.00	37.01	C
ATOM	415	CB	MET	A	383	2.425	-19.295	-2.124	1.00	37.76	C
ATOM	416	CG	MET	A	383	2.854	-18.195	-3.108	1.00	44.12	C
ATOM	417	SD	MET	A	383	4.495	-18.400	-3.806	1.00	45.79	S
ATOM	418	CE	MET	A	383	4.148	-19.720	-4.849	1.00	27.93	C
ATOM	419	C	MET	A	383	-0.054	-19.244	-2.490	1.00	33.92	C
ATOM	420	O	MET	A	383	-0.365	-18.389	-3.311	1.00	28.10	O
ATOM	421	N	MET	A	384	-0.672	-20.423	-2.432	1.00	30.29	N
ATOM	422	CA	MET	A	384	-1.770	-20.707	-3.346	1.00	35.41	C
ATOM	423	CB	MET	A	384	-2.129	-22.190	-3.338	1.00	37.28	C
ATOM	424	CG	MET	A	384	-1.098	-23.082	-4.013	1.00	44.29	C
ATOM	425	SD	MET	A	384	-0.753	-22.611	-5.733	1.00	47.70	S
ATOM	426	CE	MET	A	384	-2.394	-22.740	-6.491	1.00	43.44	C
ATOM	427	C	MET	A	384	-2.988	-19.871	-2.970	1.00	32.30	C
ATOM	428	O	MET	A	384	-3.746	-19.436	-3.838	1.00	32.40	O
ATOM	429	N	ARG	A	385	-3.186	-19.642	-1.680	1.00	36.42	N
ATOM	430	CA	ARG	A	385	-4.305	-18.814	-1.250	1.00	36.70	C
ATOM	431	CB	ARG	A	385	-4.470	-18.850	0.270	1.00	41.37	C
ATOM	432	CG	ARG	A	385	-5.158	-20.106	0.794	1.00	46.84	C
ATOM	433	CD	ARG	A	385	-5.569	-19.933	2.261	1.00	45.50	C
ATOM	434	NE	ARG	A	385	-4.432	-20.021	3.171	1.00	49.04	N
ATOM	435	CZ	ARG	A	385	-3.842	-21.165	3.508	1.00	48.50	C
ATOM	436	NH1	ARG	A	385	-4.291	-22.309	3.007	1.00	48.28	N
ATOM	437	NH2	ARG	A	385	-2.806	-21.167	4.334	1.00	48.88	N
ATOM	438	C	ARG	A	385	-4.048	-17.381	-1.712	1.00	32.36	C
ATOM	439	O	ARG	A	385	-4.970	-16.666	-2.088	1.00	34.82	O

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ATOM	440	N	GLU A 386	-2.780	-16.976	-1.692	1.00	29.93	N
ATOM	441	CA	GLU A 386	-2.395	-15.633	-2.125	1.00	29.40	C
ATOM	442	CB	GLU A 386	-0.893	-15.413	-1.881	1.00	28.50	C
ATOM	443	CG	GLU A 386	-0.333	-14.053	-2.289	1.00	33.73	C
ATOM	444	CD	GLU A 386	1.178	-13.959	-2.037	1.00	35.02	C
ATOM	445	OE1	GLU A 386	1.750	-14.956	-1.548	1.00	36.68	O
ATOM	446	OE2	GLU A 386	1.797	-12.905	-2.343	1.00	36.70	O
ATOM	447	C	GLU A 386	-2.713	-15.481	-3.615	1.00	27.47	C
ATOM	448	O	GLU A 386	-3.215	-14.437	-4.060	1.00	28.61	O
ATOM	449	N	ALA A 387	-2.412	-16.525	-4.377	1.00	30.23	N
ATOM	450	CA	ALA A 387	-2.673	-16.488	-5.806	1.00	33.30	C
ATOM	451	CB	ALA A 387	-2.097	-17.735	-6.484	1.00	32.95	C
ATOM	452	C	ALA A 387	-4.194	-16.386	-6.031	1.00	30.92	C
ATOM	453	O	ALA A 387	-4.638	-15.601	-6.843	1.00	33.56	O
ATOM	454	N	GLN A 388	-4.975	-17.163	-5.286	1.00	31.73	N
ATOM	455	CA	GLN A 388	-6.440	-17.119	-5.438	1.00	36.88	C
ATOM	456	CB	GLN A 388	-7.108	-18.109	-4.461	1.00	39.93	C
ATOM	457	CG	GLN A 388	-6.725	-19.564	-4.694	1.00	48.53	C
ATOM	458	CD	GLN A 388	-7.273	-20.496	-3.619	1.00	55.51	C
ATOM	459	OE1	GLN A 388	-8.480	-20.524	-3.360	1.00	58.01	O
ATOM	460	NE2	GLN A 388	-6.383	-21.263	-2.982	1.00	52.09	N
ATOM	461	C	GLN A 388	-7.001	-15.711	-5.201	1.00	33.60	C
ATOM	462	O	GLN A 388	-7.904	-15.271	-5.902	1.00	31.97	O
ATOM	463	N	ILE A 389	-6.469	-15.004	-4.204	1.00	30.12	N
ATOM	464	CA	ILE A 389	-6.914	-13.643	-3.905	1.00	25.06	C
ATOM	465	CB	ILE A 389	-6.305	-13.132	-2.569	1.00	28.76	C
ATOM	466	CG2	ILE A 389	-6.507	-11.626	-2.426	1.00	29.47	C
ATOM	467	CG1	ILE A 389	-6.964	-13.868	-1.398	1.00	37.06	C
ATOM	468	CD1	ILE A 389	-6.359	-13.540	-0.058	1.00	34.67	C
ATOM	469	C	ILE A 389	-6.524	-12.696	-5.022	1.00	26.55	C
ATOM	470	O	ILE A 389	-7.326	-11.901	-5.494	1.00	30.71	O
ATOM	471	N	MET A 390	-5.278	-12.779	-5.461	1.00	27.33	N
ATOM	472	CA	MET A 390	-4.845	-11.910	-6.529	1.00	24.55	C
ATOM	473	CB	MET A 390	-3.353	-12.085	-6.809	1.00	24.16	C
ATOM	474	CG	MET A 390	-2.457	-11.523	-5.714	1.00	24.68	C
ATOM	475	SD	MET A 390	-0.694	-11.770	-6.180	1.00	31.52	S
ATOM	476	CE	MET A 390	-0.450	-10.325	-7.210	1.00	31.50	C
ATOM	477	C	MET A 390	-5.638	-12.215	-7.807	1.00	29.46	C
ATOM	478	O	MET A 390	-5.960	-11.302	-8.558	1.00	30.11	O
ATOM	479	N	HIS A 391	-5.945	-13.493	-8.024	1.00	30.83	N
ATOM	480	CA	HIS A 391	-6.689	-13.890	-9.230	1.00	37.84	C
ATOM	481	CB	HIS A 391	-6.738	-15.420	-9.340	1.00	43.52	C
ATOM	482	CG	HIS A 391	-7.283	-15.921	-10.645	1.00	49.94	C
ATOM	483	CD2	HIS A 391	-6.657	-16.380	-11.756	1.00	51.86	C
ATOM	484	ND1	HIS A 391	-8.633	-15.956	-10.924	1.00	55.85	N
ATOM	485	CE1	HIS A 391	-8.816	-16.416	-12.149	1.00	57.35	C
ATOM	486	NE2	HIS A 391	-7.634	-16.681	-12.675	1.00	57.80	N
ATOM	487	C	HIS A 391	-8.106	-13.321	-9.231	1.00	42.10	C
ATOM	488	O	HIS A 391	-8.778	-13.315	-10.262	1.00	47.79	O
ATOM	489	N	GLN A 392	-8.559	-12.839	-8.077	1.00	39.91	N
ATOM	490	CA	GLN A 392	-9.898	-12.259	-7.965	1.00	41.34	C
ATOM	491	CB	GLN A 392	-10.543	-12.659	-6.633	1.00	43.83	C
ATOM	492	CG	GLN A 392	-10.631	-14.161	-6.437	1.00	47.90	C
ATOM	493	CD	GLN A 392	-11.399	-14.548	-5.197	1.00	51.89	C
ATOM	494	OE1	GLN A 392	-12.612	-14.361	-5.124	1.00	58.95	O
ATOM	495	NE2	GLN A 392	-10.699	-15.095	-4.210	1.00	51.91	N
ATOM	496	C	GLN A 392	-9.860	-10.742	-8.067	1.00	46.24	C
ATOM	497	O	GLN A 392	-10.888	-10.081	-7.932	1.00	43.30	O
ATOM	498	N	LEU A 393	-8.676	-10.190	-8.317	1.00	43.90	N
ATOM	499	CA	LEU A 393	-8.511	-8.741	-8.416	1.00	43.71	C
ATOM	500	CB	LEU A 393	-7.350	-8.287	-7.530	1.00	46.31	C
ATOM	501	CG	LEU A 393	-7.356	-8.772	-6.080	1.00	47.53	C
ATOM	502	CD1	LEU A 393	-6.097	-8.274	-5.384	1.00	44.78	C
ATOM	503	CD2	LEU A 393	-8.601	-8.278	-5.364	1.00	38.33	C
ATOM	504	C	LEU A 393	-8.269	-8.257	-9.843	1.00	45.51	C
ATOM	505	O	LEU A 393	-7.485	-8.847	-10.597	1.00	50.21	O
ATOM	506	N	ASP A 394	-8.924	-7.167	-10.220	1.00	41.60	N
ATOM	507	CA	ASP A 394	-8.759	-6.638	-11.565	1.00	38.62	C

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ATOM   508  CB   ASP A 394      -9.874  -7.175 -12.473  1.00 45.48           C
ATOM   509  CG   ASP A 394      -9.733  -6.718 -13.917  1.00 53.93           C
ATOM   510  OD1  ASP A 394     -10.609  -7.075 -14.740  1.00 54.65           O
ATOM   511  OD2  ASP A 394      -8.756  -6.009 -14.235  1.00 49.40           O
ATOM   512  C    ASP A 394      -8.821  -5.132 -11.499  1.00 41.64           C
ATOM   513  O    ASP A 394      -9.870  -4.523 -11.744  1.00 41.10           O
ATOM   514  N    ASN A 395      -7.692  -4.519 -11.169  1.00 38.06           N
ATOM   515  CA   ASN A 395      -7.654  -3.075 -11.057  1.00 29.93           C
ATOM   516  CB   ASN A 395      -7.902  -2.678  -9.592  1.00 27.46           C
ATOM   517  CG   ASN A 395      -8.027  -1.187  -9.397  1.00 34.86           C
ATOM   518  OD1  ASN A 395      -9.106  -0.602  -9.581  1.00 38.20           O
ATOM   519  ND2  ASN A 395      -6.923  -0.552  -9.025  1.00 25.87           N
ATOM   520  C    ASN A 395      -6.285  -2.610 -11.530  1.00 30.95           C
ATOM   521  O    ASN A 395      -5.258  -3.260 -11.269  1.00 28.17           O
ATOM   522  N    PRO A 396      -6.248  -1.467 -12.222  1.00 28.97           N
ATOM   523  CD   PRO A 396      -7.395  -0.706 -12.748  1.00 39.56           C
ATOM   524  CA   PRO A 396      -4.996  -0.919 -12.733  1.00 28.79           C
ATOM   525  CB   PRO A 396      -5.464   0.277 -13.556  1.00 37.29           C
ATOM   526  CG   PRO A 396      -6.842  -0.149 -14.019  1.00 42.13           C
ATOM   527  C    PRO A 396      -3.997  -0.494 -11.656  1.00 28.11           C
ATOM   528  O    PRO A 396      -2.821  -0.352 -11.939  1.00 27.45           O
ATOM   529  N    TYR A 397      -4.471  -0.298 -10.422  1.00 24.07           N
ATOM   530  CA   TYR A 397      -3.576   0.171  -9.346  1.00 22.72           C
ATOM   531  CB   TYR A 397      -4.250   1.346  -8.618  1.00 21.97           C
ATOM   532  CG   TYR A 397      -4.655   2.442  -9.593  1.00 25.66           C
ATOM   533  CD1  TYR A 397      -5.994   2.640  -9.946  1.00 29.62           C
ATOM   534  CE1  TYR A 397      -6.356   3.604 -10.886  1.00 34.32           C
ATOM   535  CD2  TYR A 397      -3.689   3.238 -10.206  1.00 25.78           C
ATOM   536  CE2  TYR A 397      -4.044   4.206 -11.152  1.00 36.01           C
ATOM   537  CZ   TYR A 397      -5.376   4.380 -11.490  1.00 37.11           C
ATOM   538  OH   TYR A 397      -5.694   5.301 -12.473  1.00 40.47           O
ATOM   539  C    TYR A 397      -3.127  -0.896  -8.368  1.00 21.63           C
ATOM   540  O    TYR A 397      -2.730  -0.615  -7.213  1.00 23.29           O
ATOM   541  N    ILE A 398      -3.193  -2.125  -8.832  1.00 22.86           N
ATOM   542  CA   ILE A 398      -2.770  -3.266  -8.069  1.00 29.14           C
ATOM   543  CB   ILE A 398      -4.005  -4.065  -7.641  1.00 34.44           C
ATOM   544  CG2  ILE A 398      -3.602  -5.424  -7.156  1.00 37.06           C
ATOM   545  CG1  ILE A 398      -4.768  -3.273  -6.575  1.00 28.40           C
ATOM   546  CD1  ILE A 398      -6.166  -3.759  -6.305  1.00 41.40           C
ATOM   547  C    ILE A 398      -1.858  -4.102  -8.975  1.00 33.99           C
ATOM   548  O    ILE A 398      -2.096  -4.193 -10.183  1.00 34.40           O
ATOM   549  N    VAL A 399      -0.805  -4.672  -8.402  1.00 27.19           N
ATOM   550  CA   VAL A 399       0.109  -5.540  -9.155  1.00 26.99           C
ATOM   551  CB   VAL A 399       1.298  -6.006  -8.302  1.00 29.43           C
ATOM   552  CG1  VAL A 399       2.078  -7.146  -9.026  1.00 26.20           C
ATOM   553  CG2  VAL A 399       2.200  -4.832  -8.031  1.00 30.03           C
ATOM   554  C    VAL A 399      -0.704  -6.759  -9.539  1.00 33.87           C
ATOM   555  O    VAL A 399      -1.162  -7.498  -8.670  1.00 35.03           O
ATOM   556  N    ARG A 400      -0.849  -6.986 -10.837  1.00 26.00           N
ATOM   557  CA   ARG A 400      -1.652  -8.098 -11.315  1.00 30.60           C
ATOM   558  CB   ARG A 400      -2.172  -7.785 -12.728  1.00 38.54           C
ATOM   559  CG   ARG A 400      -3.035  -6.521 -12.854  1.00 46.40           C
ATOM   560  CD   ARG A 400      -3.410  -6.240 -14.331  1.00 46.44           C
ATOM   561  NE   ARG A 400      -4.269  -5.066 -14.505  1.00 52.85           N
ATOM   562  CZ   ARG A 400      -5.554  -5.032 -14.163  1.00 56.01           C
ATOM   563  NH1  ARG A 400      -6.117  -6.110 -13.633  1.00 52.93           N
ATOM   564  NH2  ARG A 400      -6.276  -3.928 -14.346  1.00 53.59           N
ATOM   565  C    ARG A 400      -0.946  -9.444 -11.324  1.00 27.57           C
ATOM   566  O    ARG A 400       0.257  -9.548 -11.572  1.00 27.90           O
ATOM   567  N    LEU A 401      -1.703 -10.500 -11.077  1.00 28.32           N
ATOM   568  CA   LEU A 401      -1.147 -11.838 -11.096  1.00 24.81           C
ATOM   569  CB   LEU A 401      -1.974 -12.777 -10.238  1.00 32.19           C
ATOM   570  CG   LEU A 401      -1.534 -14.239 -10.271  1.00 29.13           C
ATOM   571  CD1  LEU A 401      -0.159 -14.414  -9.638  1.00 37.61           C
ATOM   572  CD2  LEU A 401      -2.578 -15.046  -9.516  1.00 42.15           C
ATOM   573  C    LEU A 401      -1.194 -12.352 -12.525  1.00 32.86           C
ATOM   574  O    LEU A 401      -2.248 -12.281 -13.176  1.00 30.25           O
ATOM   575  N    ILE A 402      -0.060 -12.831 -13.026  1.00 26.16           N
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ATOM	576	CA	ILE	A	402	-0.031	-13.405	-14.364	1.00 28.41
ATOM	577	CB	ILE	A	402	1.394	-13.397	-14.987	1.00 29.05
ATOM	578	CG2	ILE	A	402	1.360	-14.080	-16.360	1.00 33.43
ATOM	579	CG1	ILE	A	402	1.898	-11.957	-15.135	1.00 28.86
ATOM	580	CD1	ILE	A	402	0.925	-11.026	-15.810	1.00 33.60
ATOM	581	C	ILE	A	402	-0.508	-14.853	-14.187	1.00 31.32
ATOM	582	O	ILE	A	402	-1.402	-15.330	-14.890	1.00 29.93
ATOM	583	N	GLY	A	403	0.070	-15.548	-13.224	1.00 29.11
ATOM	584	CA	GLY	A	403	-0.335	-16.924	-12.971	1.00 28.71
ATOM	585	C	GLY	A	403	0.639	-17.626	-12.060	1.00 29.89
ATOM	586	O	GLY	A	403	1.605	-17.020	-11.612	1.00 29.79
ATOM	587	N	VAL	A	404	0.387	-18.900	-11.787	1.00 27.61
ATOM	588	CA	VAL	A	404	1.259	-19.697	-10.938	1.00 31.08
ATOM	589	CB	VAL	A	404	0.436	-20.508	-9.911	1.00 36.46
ATOM	590	CG1	VAL	A	404	1.360	-21.378	-9.052	1.00 42.77
ATOM	591	CG2	VAL	A	404	-0.370	-19.564	-9.051	1.00 37.69
ATOM	592	C	VAL	A	404	2.019	-20.671	-11.823	1.00 29.99
ATOM	593	O	VAL	A	404	1.480	-21.154	-12.802	1.00 32.94
ATOM	594	N	CYS	A	405	3.262	-20.969	-11.461	1.00 31.70
ATOM	595	CA	CYS	A	405	4.065	-21.908	-12.243	1.00 37.20
ATOM	596	CB	CYS	A	405	5.131	-21.150	-13.042	1.00 40.22
ATOM	597	SG	CYS	A	405	5.968	-22.154	-14.282	1.00 46.07
ATOM	598	C	CYS	A	405	4.717	-22.939	-11.324	1.00 40.66
ATOM	599	O	CYS	A	405	5.428	-22.587	-10.388	1.00 39.23
ATOM	600	N	GLN	A	406	4.453	-24.213	-11.583	1.00 40.69
ATOM	601	CA	GLN	A	406	5.011	-25.282	-10.762	1.00 50.34
ATOM	602	CB	GLN	A	406	3.900	-26.245	-10.326	1.00 53.46
ATOM	603	CG	GLN	A	406	4.373	-27.437	-9.486	1.00 59.61
ATOM	604	CD	GLN	A	406	5.156	-27.032	-8.240	1.00 55.65
ATOM	605	OE1	GLN	A	406	6.329	-26.665	-8.316	1.00 61.62
ATOM	606	NE2	GLN	A	406	4.504	-27.099	-7.088	1.00 58.42
ATOM	607	C	GLN	A	406	6.090	-26.044	-11.519	1.00 53.49
ATOM	608	O	GLN	A	406	5.792	-26.902	-12.345	1.00 56.41
ATOM	609	N	ALA	A	407	7.342	-25.718	-11.234	1.00 54.94
ATOM	610	CA	ALA	A	407	8.468	-26.378	-11.879	1.00 59.69
ATOM	611	CB	ALA	A	407	9.105	-25.437	-12.902	1.00 59.62
ATOM	612	C	ALA	A	407	9.484	-26.782	-10.811	1.00 57.77
ATOM	613	O	ALA	A	407	9.173	-27.578	-9.923	1.00 57.65
ATOM	614	N	GLU	A	408	10.692	-26.232	-10.895	1.00 54.86
ATOM	615	CA	GLU	A	408	11.730	-26.541	-9.921	1.00 56.21
ATOM	616	CB	GLU	A	408	13.002	-25.738	-10.220	1.00 60.73
ATOM	617	CG	GLU	A	408	12.777	-24.237	-10.370	1.00 60.37
ATOM	618	CD	GLU	A	408	12.597	-23.801	-11.818	1.00 61.95
ATOM	619	OE1	GLU	A	408	11.749	-24.377	-12.535	1.00 61.59
ATOM	620	OE2	GLU	A	408	13.308	-22.866	-12.238	1.00 60.74
ATOM	621	C	GLU	A	408	11.216	-26.210	-8.524	1.00 57.49
ATOM	622	O	GLU	A	408	11.766	-26.663	-7.517	1.00 60.01
ATOM	623	N	ALA	A	409	10.155	-25.411	-8.480	1.00 56.44
ATOM	624	CA	ALA	A	409	9.519	-25.007	-7.231	1.00 52.91
ATOM	625	CB	ALA	A	409	10.480	-24.178	-6.392	1.00 58.00
ATOM	626	C	ALA	A	409	8.276	-24.196	-7.589	1.00 49.70
ATOM	627	O	ALA	A	409	8.092	-23.822	-8.750	1.00 46.56
ATOM	628	N	LEU	A	410	7.420	-23.942	-6.601	1.00 48.39
ATOM	629	CA	LEU	A	410	6.189	-23.192	-6.830	1.00 42.60
ATOM	630	CB	LEU	A	410	5.210	-23.433	-5.681	1.00 42.05
ATOM	631	CG	LEU	A	410	3.794	-22.949	-5.968	1.00 39.06
ATOM	632	CD1	LEU	A	410	3.256	-23.669	-7.199	1.00 42.72
ATOM	633	CD2	LEU	A	410	2.912	-23.207	-4.752	1.00 46.20
ATOM	634	C	LEU	A	410	6.516	-21.711	-6.941	1.00 34.88
ATOM	635	O	LEU	A	410	7.246	-21.174	-6.118	1.00 32.97
ATOM	636	N	MET	A	411	5.969	-21.052	-7.956	1.00 32.78
ATOM	637	CA	MET	A	411	6.269	-19.647	-8.171	1.00 27.80
ATOM	638	CB	MET	A	411	7.272	-19.506	-9.326	1.00 29.67
ATOM	639	CG	MET	A	411	8.546	-20.333	-9.200	1.00 37.85
ATOM	640	SD	MET	A	411	9.647	-20.153	-10.644	1.00 40.33
ATOM	641	CE	MET	A	411	8.672	-20.909	-11.859	1.00 38.19
ATOM	642	C	MET	A	411	5.024	-18.846	-8.521	1.00 29.61
ATOM	643	O	MET	A	411	4.126	-19.354	-9.171	1.00 32.53

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                                      atomic coordinates.txt
ATOM    644  N   LEU A 412        4.975 -17.593  -8.083  1.00 26.11          N
ATOM    645  CA  LEU A 412        3.864 -16.704  -8.426  1.00 23.60          C
ATOM    646  CB  LEU A 412        3.340 -15.957  -7.197  1.00 30.66          C
ATOM    647  CG  LEU A 412        2.475 -16.741  -6.224  1.00 43.14          C
ATOM    648  CD1 LEU A 412        1.856 -15.774  -5.208  1.00 39.76          C
ATOM    649  CD2 LEU A 412        1.389 -17.457  -7.018  1.00 42.58          C
ATOM    650  C   LEU A 412        4.450 -15.688  -9.391  1.00 33.31          C
ATOM    651  O   LEU A 412        5.348 -14.947  -9.004  1.00 24.93          O
ATOM    652  N   VAL A 413        3.928 -15.663 -10.626  1.00 26.19          N
ATOM    653  CA  VAL A 413        4.385 -14.739 -11.674  1.00 24.01          C
ATOM    654  CB  VAL A 413        4.374 -15.425 -13.070  1.00 25.63          C
ATOM    655  CG1 VAL A 413        4.951 -14.465 -14.143  1.00 22.85          C
ATOM    656  CG2 VAL A 413        5.192 -16.718 -13.010  1.00 26.67          C
ATOM    657  C   VAL A 413        3.458 -13.540 -11.700  1.00 26.19          C
ATOM    658  O   VAL A 413        2.240 -13.673 -11.925  1.00 28.56          O
ATOM    659  N   MET A 414        4.052 -12.368 -11.490  1.00 22.49          N
ATOM    660  CA  MET A 414        3.324 -11.108 -11.418  1.00 22.14          C
ATOM    661  CB  MET A 414        3.422 -10.545  -9.987  1.00 25.30          C
ATOM    662  CG  MET A 414        2.767 -11.409  -8.917  1.00 28.88          C
ATOM    663  SD  MET A 414        3.377 -10.874  -7.264  1.00 30.85          S
ATOM    664  CE  MET A 414        4.890 -11.872  -7.109  1.00 32.45          C
ATOM    665  C   MET A 414        3.871 -10.049 -12.336  1.00 24.63          C
ATOM    666  O   MET A 414        5.017 -10.131 -12.796  1.00 25.46          O
ATOM    667  N   GLU A 415        3.075  -9.012 -12.568  1.00 25.97          N
ATOM    668  CA  GLU A 415        3.548  -7.913 -13.395  1.00 25.91          C
ATOM    669  CB  GLU A 415        2.470  -6.842 -13.568  1.00 37.31          C
ATOM    670  CG  GLU A 415        1.181  -7.321 -14.191  1.00 41.51          C
ATOM    671  CD  GLU A 415        0.151  -6.190 -14.258  1.00 56.50          C
ATOM    672  OE1 GLU A 415       -0.056  -5.493 -13.222  1.00 39.84          O
ATOM    673  OE2 GLU A 415       -0.444  -5.998 -15.346  1.00 55.15          O
ATOM    674  C   GLU A 415        4.711  -7.273 -12.651  1.00 26.45          C
ATOM    675  O   GLU A 415        4.751  -7.287 -11.417  1.00 26.92          O
ATOM    676  N   MET A 416        5.657  -6.713 -13.400  1.00 27.12          N
ATOM    677  CA  MET A 416        6.784  -6.047 -12.778  1.00 26.18          C
ATOM    678  CB  MET A 416        8.078  -6.343 -13.519  1.00 29.98          C
ATOM    679  CG  MET A 416        9.308  -5.885 -12.729  1.00 32.43          C
ATOM    680  SD  MET A 416       10.835  -6.141 -13.631  1.00 40.73          S
ATOM    681  CE  MET A 416       11.931  -4.939 -12.809  1.00 40.48          C
ATOM    682  C   MET A 416        6.577  -4.539 -12.781  1.00 30.68          C
ATOM    683  O   MET A 416        6.117  -3.981 -13.766  1.00 29.07          O
ATOM    684  N   ALA A 417        6.916  -3.893 -11.670  1.00 28.26          N
ATOM    685  CA  ALA A 417        6.843  -2.436 -11.561  1.00 31.40          C
ATOM    686  CB  ALA A 417        5.886  -2.019 -10.435  1.00 31.37          C
ATOM    687  C   ALA A 417        8.286  -2.023 -11.253  1.00 31.10          C
ATOM    688  O   ALA A 417        8.672  -1.865 -10.087  1.00 31.97          O
ATOM    689  N   GLY A 418        9.064  -1.876 -12.330  1.00 35.10          N
ATOM    690  CA  GLY A 418       10.485  -1.554 -12.258  1.00 34.74          C
ATOM    691  C   GLY A 418       10.936  -0.340 -11.474  1.00 32.22          C
ATOM    692  O   GLY A 418       12.120  -0.205 -11.147  1.00 33.36          O
ATOM    693  N   GLY A 419       10.002   0.559 -11.183  1.00 26.94          N
ATOM    694  CA  GLY A 419       10.354   1.740 -10.421  1.00 27.31          C
ATOM    695  C   GLY A 419       10.674   1.386  -8.978  1.00 32.93          C
ATOM    696  O   GLY A 419       11.321   2.150  -8.287  1.00 31.61          O
ATOM    697  N   GLY A 420       10.196   0.235  -8.506  1.00 32.29          N
ATOM    698  CA  GLY A 420       10.469  -0.166  -7.139  1.00 27.34          C
ATOM    699  C   GLY A 420        9.632   0.511  -6.054  1.00 27.22          C
ATOM    700  O   GLY A 420        8.709   1.263  -6.369  1.00 25.34          O
ATOM    701  N   PRO A 421        9.952   0.280  -4.770  1.00 27.85          N
ATOM    702  CD  PRO A 421       11.122  -0.509  -4.330  1.00 29.71          C
ATOM    703  CA  PRO A 421        9.247   0.843  -3.612  1.00 25.99          C
ATOM    704  CB  PRO A 421       10.049   0.310  -2.411  1.00 33.47          C
ATOM    705  CG  PRO A 421       10.755  -0.872  -2.921  1.00 33.83          C
ATOM    706  C   PRO A 421        9.178   2.358  -3.574  1.00 32.23          C
ATOM    707  O   PRO A 421       10.162   3.052  -3.845  1.00 25.70          O
ATOM    708  N   LEU A 422        8.002   2.856  -3.196  1.00 24.75          N
ATOM    709  CA  LEU A 422        7.726   4.280  -3.094  1.00 24.74          C
ATOM    710  CB  LEU A 422        6.258   4.475  -2.705  1.00 25.86          C
ATOM    711  CG  LEU A 422        5.736   5.899  -2.536  1.00 27.46          C
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ATOM    712  CD1 LEU A 422      5.749   6.599  -3.879  1.00 29.48           C
ATOM    713  CD2 LEU A 422      4.322   5.851  -1.989  1.00 26.17           C
ATOM    714  C   LEU A 422      8.607   5.010  -2.078  1.00 24.09           C
ATOM    715  O   LEU A 422      9.065   6.128  -2.347  1.00 27.09           O
ATOM    716  N   HIS A 423      8.821   4.423  -0.908  1.00 23.84           N
ATOM    717  CA  HIS A 423      9.627   5.097   0.097  1.00 31.59           C
ATOM    718  CB  HIS A 423      9.677   4.309   1.410  1.00 33.34           C
ATOM    719  CG  HIS A 423     10.255   2.935   1.274  1.00 32.56           C
ATOM    720  CD2 HIS A 423     10.263   2.066   0.236  1.00 33.97           C
ATOM    721  ND1 HIS A 423     10.947   2.318   2.296  1.00 40.55           N
ATOM    722  CE1 HIS A 423     11.355   1.128   1.894  1.00 33.85           C
ATOM    723  NE2 HIS A 423     10.952   0.950   0.647  1.00 37.19           N
ATOM    724  C   HIS A 423     11.048   5.352  -0.417  1.00 35.72           C
ATOM    725  O   HIS A 423     11.583   6.444  -0.235  1.00 38.98           O
ATOM    726  N   LYS A 424     11.647   4.356  -1.064  1.00 26.67           N
ATOM    727  CA  LYS A 424     13.000   4.559  -1.576  1.00 30.40           C
ATOM    728  CB  LYS A 424     13.625   3.217  -1.950  1.00 30.75           C
ATOM    729  CG  LYS A 424     13.884   2.327  -0.747  1.00 32.42           C
ATOM    730  CD  LYS A 424     14.486   0.996  -1.191  1.00 42.37           C
ATOM    731  CE  LYS A 424     14.635   0.035  -0.020  1.00 47.25           C
ATOM    732  NZ  LYS A 424     15.606  -1.054  -0.360  1.00 54.40           N
ATOM    733  C   LYS A 424     13.025   5.500  -2.767  1.00 30.87           C
ATOM    734  O   LYS A 424     13.976   6.259  -2.944  1.00 27.95           O
ATOM    735  N   PHE A 425     11.975   5.479  -3.586  1.00 27.56           N
ATOM    736  CA  PHE A 425     11.919   6.345  -4.755  1.00 27.56           C
ATOM    737  CB  PHE A 425     10.693   6.006  -5.612  1.00 33.85           C
ATOM    738  CG  PHE A 425     10.536   6.885  -6.816  1.00 33.08           C
ATOM    739  CD1 PHE A 425     11.259   6.634  -7.976  1.00 43.47           C
ATOM    740  CD2 PHE A 425      9.692   7.986  -6.778  1.00 38.10           C
ATOM    741  CE1 PHE A 425     11.146   7.473  -9.083  1.00 42.11           C
ATOM    742  CE2 PHE A 425      9.567   8.832  -7.874  1.00 47.88           C
ATOM    743  CZ  PHE A 425     10.297   8.574  -9.033  1.00 44.70           C
ATOM    744  C   PHE A 425     11.861   7.838  -4.391  1.00 29.42           C
ATOM    745  O   PHE A 425     12.421   8.681  -5.097  1.00 28.17           O
ATOM    746  N   LEU A 426     11.198   8.174  -3.295  1.00 26.78           N
ATOM    747  CA  LEU A 426     11.053   9.581  -2.919  1.00 23.65           C
ATOM    748  CB  LEU A 426      9.750   9.793  -2.142  1.00 23.99           C
ATOM    749  CG  LEU A 426      8.484   9.534  -2.972  1.00 23.37           C
ATOM    750  CD1 LEU A 426      7.234   9.646  -2.081  1.00 23.77           C
ATOM    751  CD2 LEU A 426      8.429  10.547  -4.096  1.00 27.33           C
ATOM    752  C   LEU A 426     12.210  10.161  -2.100  1.00 29.71           C
ATOM    753  O   LEU A 426     12.345  11.379  -2.011  1.00 24.55           O
ATOM    754  N   VAL A 427     13.021   9.296  -1.501  1.00 25.47           N
ATOM    755  CA  VAL A 427     14.130   9.781  -0.661  1.00 28.99           C
ATOM    756  CB  VAL A 427     14.996   8.607  -0.132  1.00 34.76           C
ATOM    757  CG1 VAL A 427     16.250   9.148   0.578  1.00 37.93           C
ATOM    758  CG2 VAL A 427     14.186   7.762   0.852  1.00 30.76           C
ATOM    759  C   VAL A 427     15.027  10.780  -1.403  1.00 34.84           C
ATOM    760  O   VAL A 427     15.605  10.464  -2.445  1.00 37.55           O
ATOM    761  N   GLY A 428     15.117  11.993  -0.862  1.00 43.08           N
ATOM    762  CA  GLY A 428     15.941  13.030  -1.469  1.00 41.65           C
ATOM    763  C   GLY A 428     15.437  13.634  -2.768  1.00 47.74           C
ATOM    764  O   GLY A 428     16.196  14.303  -3.479  1.00 42.77           O
ATOM    765  N   LYS A 429     14.163  13.430  -3.090  1.00 37.30           N
ATOM    766  CA  LYS A 429     13.624  13.972  -4.328  1.00 41.14           C
ATOM    767  CB  LYS A 429     13.024  12.840  -5.161  1.00 46.03           C
ATOM    768  CG  LYS A 429     14.064  11.799  -5.568  1.00 46.82           C
ATOM    769  CD  LYS A 429     13.607  11.007  -6.775  1.00 54.33           C
ATOM    770  CE  LYS A 429     14.575   9.879  -7.099  1.00 52.59           C
ATOM    771  NZ  LYS A 429     14.028   9.018  -8.182  1.00 61.02           N
ATOM    772  C   LYS A 429     12.596  15.079  -4.098  1.00 43.46           C
ATOM    773  O   LYS A 429     11.741  15.347  -4.952  1.00 46.64           O
ATOM    774  N   ARG A 430     12.696  15.736  -2.950  1.00 38.34           N
ATOM    775  CA  ARG A 430     11.765  16.798  -2.604  1.00 51.71           C
ATOM    776  CB  ARG A 430     12.050  17.298  -1.189  1.00 53.36           C
ATOM    777  CG  ARG A 430     10.922  18.125  -0.591  1.00 62.96           C
ATOM    778  CD  ARG A 430     11.039  18.217   0.928  1.00 63.14           C
ATOM    779  NE  ARG A 430      9.729  18.100   1.576  1.00 62.24           N
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ATOM    780  CZ   ARG A 430      9.526  17.461   2.724  1.00 68.34           C
ATOM    781  NH1  ARG A 430     10.545  16.890   3.355  1.00 63.91           N
ATOM    782  NH2  ARG A 430      8.293  17.358   3.231  1.00 65.90           N
ATOM    783  C    ARG A 430     11.818  17.957  -3.591  1.00 54.65           C
ATOM    784  O    ARG A 430     10.867  18.723  -3.716  1.00 53.09           O
ATOM    785  N    GLU A 431     12.932  18.078  -4.307  1.00 55.81           N
ATOM    786  CA   GLU A 431     13.077  19.158  -5.268  1.00 54.84           C
ATOM    787  CB   GLU A 431     14.428  19.855  -5.092  1.00 58.53           C
ATOM    788  CG   GLU A 431     14.491  20.755  -3.869  1.00 61.42           C
ATOM    789  CD   GLU A 431     15.662  21.716  -3.910  1.00 67.37           C
ATOM    790  OE1  GLU A 431     15.715  22.555  -4.841  1.00 71.67           O
ATOM    791  OE2  GLU A 431     16.530  21.638  -3.013  1.00 68.85           O
ATOM    792  C    GLU A 431     12.913  18.709  -6.705  1.00 55.28           C
ATOM    793  O    GLU A 431     12.995  19.521  -7.622  1.00 58.15           O
ATOM    794  N    GLU A 432     12.678  17.420  -6.912  1.00 50.44           N
ATOM    795  CA   GLU A 432     12.498  16.923  -8.263  1.00 48.35           C
ATOM    796  CB   GLU A 432     13.596  15.918  -8.623  1.00 55.95           C
ATOM    797  CG   GLU A 432     13.285  14.477  -8.287  1.00 59.72           C
ATOM    798  CD   GLU A 432     14.264  13.513  -8.934  1.00 62.60           C
ATOM    799  OE1  GLU A 432     15.463  13.571  -8.594  1.00 66.37           O
ATOM    800  OE2  GLU A 432     13.837  12.700  -9.786  1.00 65.64           O
ATOM    801  C    GLU A 432     11.125  16.285  -8.432  1.00 47.94           C
ATOM    802  O    GLU A 432     10.661  16.082  -9.548  1.00 47.37           O
ATOM    803  N    ILE A 433     10.474  15.968  -7.315  1.00 39.35           N
ATOM    804  CA   ILE A 433      9.143  15.364  -7.361  1.00 35.26           C
ATOM    805  CB   ILE A 433      9.148  13.942  -6.758  1.00 40.43           C
ATOM    806  CG2  ILE A 433      7.742  13.332  -6.819  1.00 32.65           C
ATOM    807  CG1  ILE A 433     10.120  13.056  -7.527  1.00 39.75           C
ATOM    808  CD1  ILE A 433      9.720  12.837  -8.964  1.00 41.51           C
ATOM    809  C    ILE A 433      8.252  16.258  -6.521  1.00 36.84           C
ATOM    810  O    ILE A 433      8.276  16.182  -5.291  1.00 32.85           O
ATOM    811  N    PRO A 434      7.467  17.134  -7.172  1.00 33.02           N
ATOM    812  CD   PRO A 434      7.510  17.400  -8.618  1.00 41.68           C
ATOM    813  CA   PRO A 434      6.554  18.074  -6.512  1.00 36.57           C
ATOM    814  CB   PRO A 434      5.925  18.812  -7.693  1.00 37.02           C
ATOM    815  CG   PRO A 434      7.033  18.833  -8.679  1.00 47.39           C
ATOM    816  C    PRO A 434      5.512  17.377  -5.648  1.00 31.45           C
ATOM    817  O    PRO A 434      5.227  16.199  -5.848  1.00 28.84           O
ATOM    818  N    VAL A 435      4.944  18.121  -4.702  1.00 32.88           N
ATOM    819  CA   VAL A 435      3.919  17.568  -3.821  1.00 34.12           C
ATOM    820  CB   VAL A 435      3.457  18.619  -2.777  1.00 32.16           C
ATOM    821  CG1  VAL A 435      2.335  18.041  -1.904  1.00 32.92           C
ATOM    822  CG2  VAL A 435      4.629  19.012  -1.901  1.00 39.50           C
ATOM    823  C    VAL A 435      2.731  17.093  -4.642  1.00 34.03           C
ATOM    824  O    VAL A 435      2.096  16.076  -4.299  1.00 26.73           O
ATOM    825  N    SER A 436      2.424  17.821  -5.721  1.00 27.34           N
ATOM    826  CA   SER A 436      1.321  17.445  -6.595  1.00 26.52           C
ATOM    827  CB   SER A 436      1.152  18.482  -7.725  1.00 34.16           C
ATOM    828  OG   SER A 436      2.339  18.588  -8.494  1.00 36.95           O
ATOM    829  C    SER A 436      1.517  16.038  -7.187  1.00 29.26           C
ATOM    830  O    SER A 436      0.548  15.298  -7.359  1.00 28.55           O
ATOM    831  N    ASN A 437      2.763  15.676  -7.486  1.00 24.99           N
ATOM    832  CA   ASN A 437      3.085  14.372  -8.060  1.00 24.95           C
ATOM    833  CB   ASN A 437      4.499  14.432  -8.649  1.00 30.76           C
ATOM    834  CG.  ASN A 437      4.891  13.192  -9.462  1.00 33.40           C
ATOM    835  OD1  ASN A 437      5.922  13.209 -10.140  1.00 31.35           O
ATOM    836  ND2  ASN A 437      4.107  12.116  -9.381  1.00 33.64           N
ATOM    837  C    ASN A 437      2.957  13.330  -6.923  1.00 24.92           C
ATOM    838  O    ASN A 437      2.472  12.224  -7.133  1.00 26.65           O
ATOM    839  N    VAL A 438      3.371  13.695  -5.719  1.00 25.75           N
ATOM    840  CA   VAL A 438      3.201  12.755  -4.612  1.00 24.63           C
ATOM    841  CB   VAL A 438      3.819  13.291  -3.321  1.00 28.75           C
ATOM    842  CG1  VAL A 438      3.496  12.348  -2.162  1.00 25.61           C
ATOM    843  CG2  VAL A 438      5.338  13.426  -3.500  1.00 27.56           C
ATOM    844  C    VAL A 438      1.697  12.523  -4.409  1.00 24.68           C
ATOM    845  O    VAL A 438      1.277  11.391  -4.258  1.00 22.54           O
ATOM    846  N    ALA A 439      0.888  13.591  -4.441  1.00 22.86           N
ATOM    847  CA   ALA A 439     -0.567  13.437  -4.280  1.00 25.85           C
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ATOM	848	CB	ALA	A	439	-1.263	14.843	-4.217	1.00	25.16	C
ATOM	849	C	ALA	A	439	-1.188	12.589	-5.395	1.00	22.87	C
ATOM	850	O	ALA	A	439	-2.146	11.861	-5.154	1.00	23.17	O
ATOM	851	N	GLU	A	440	-0.647	12.685	-6.614	1.00	21.21	N
ATOM	852	CA	GLU	A	440	-1.157	11.900	-7.728	1.00	25.32	C
ATOM	853	CB	GLU	A	440	-0.380	12.246	-9.014	1.00	30.55	C
ATOM	854	CG	GLU	A	440	-0.636	11.301	-10.184	1.00	29.05	C
ATOM	855	CD	GLU	A	440	0.286	11.582	-11.368	1.00	40.39	C
ATOM	856	OE1	GLU	A	440	1.448	11.984	-11.145	1.00	35.18	O
ATOM	857	OE2	GLU	A	440	-0.151	11.385	-12.523	1.00	36.07	O
ATOM	858	C	GLU	A	440	-0.998	10.404	-7.406	1.00	31.15	C
ATOM	859	O	GLU	A	440	-1.923	9.614	-7.585	1.00	23.98	O
ATOM	860	N	LEU	A	441	0.181	10.035	-6.913	1.00	24.24	N
ATOM	861	CA	LEU	A	441	0.500	8.646	-6.573	1.00	21.78	C
ATOM	862	CB	LEU	A	441	1.991	8.541	-6.222	1.00	22.41	C
ATOM	863	CG	LEU	A	441	2.937	8.916	-7.366	1.00	22.95	C
ATOM	864	CD1	LEU	A	441	4.389	8.882	-6.901	1.00	27.25	C
ATOM	865	CD2	LEU	A	441	2.720	7.939	-8.521	1.00	19.84	C
ATOM	866	C	LEU	A	441	-0.354	8.186	-5.377	1.00	18.04	C
ATOM	867	O	LEU	A	441	-0.872	7.067	-5.375	1.00	23.44	O
ATOM	868	N	LEU	A	442	-0.476	9.040	-4.369	1.00	20.94	N
ATOM	869	CA	LEU	A	442	-1.310	8.653	-3.219	1.00	24.86	C
ATOM	870	CB	LEU	A	442	-1.233	9.698	-2.115	1.00	22.54	C
ATOM	871	CG	LEU	A	442	0.100	9.753	-1.362	1.00	22.80	C
ATOM	872	CD1	LEU	A	442	0.125	10.921	-0.355	1.00	22.67	C
ATOM	873	CD2	LEU	A	442	0.315	8.398	-0.661	1.00	23.13	C
ATOM	874	C	LEU	A	442	-2.761	8.469	-3.667	1.00	25.24	C
ATOM	875	O	LEU	A	442	-3.454	7.581	-3.187	1.00	22.68	O
ATOM	876	N	HIS	A	443	-3.228	9.290	-4.605	1.00	23.39	N
ATOM	877	CA	HIS	A	443	-4.607	9.115	-5.069	1.00	22.12	C
ATOM	878	CB	HIS	A	443	-5.024	10.280	-5.985	1.00	27.77	C
ATOM	879	CG	HIS	A	443	-6.388	10.101	-6.573	1.00	28.68	C
ATOM	880	CD2	HIS	A	443	-7.565	9.739	-6.004	1.00	27.01	C
ATOM	881	ND1	HIS	A	443	-6.628	10.196	-7.929	1.00	24.79	N
ATOM	882	CE1	HIS	A	443	-7.893	9.897	-8.171	1.00	24.33	C
ATOM	883	NE2	HIS	A	443	-8.484	9.613	-7.021	1.00	22.99	N
ATOM	884	C	HIS	A	443	-4.781	7.762	-5.781	1.00	22.67	C
ATOM	885	O	HIS	A	443	-5.792	7.077	-5.600	1.00	21.81	O
ATOM	886	N	GLN	A	444	-3.791	7.354	-6.569	1.00	22.84	N
ATOM	887	CA	GLN	A	444	-3.855	6.076	-7.251	1.00	18.98	C
ATOM	888	CB	GLN	A	444	-2.637	5.909	-8.152	1.00	23.77	C
ATOM	889	CG	GLN	A	444	-2.679	6.923	-9.303	1.00	23.82	C
ATOM	890	CD	GLN	A	444	-1.445	6.867	-10.130	1.00	29.64	C
ATOM	891	OE1	GLN	A	444	-0.424	6.344	-9.697	1.00	28.87	O
ATOM	892	NE2	GLN	A	444	-1.521	7.419	-11.342	1.00	28.75	N
ATOM	893	C	GLN	A	444	-3.911	4.958	-6.218	1.00	21.47	C
ATOM	894	O	GLN	A	444	-4.682	4.029	-6.354	1.00	22.83	O
ATOM	895	N	VAL	A	445	-3.114	5.094	-5.162	1.00	21.95	N
ATOM	896	CA	VAL	A	445	-3.162	4.075	-4.119	1.00	19.79	C
ATOM	897	CB	VAL	A	445	-2.131	4.359	-3.001	1.00	21.17	C
ATOM	898	CG1	VAL	A	445	-2.309	3.326	-1.862	1.00	22.83	C
ATOM	899	CG2	VAL	A	445	-0.732	4.274	-3.575	1.00	19.35	C
ATOM	900	C	VAL	A	445	-4.576	4.070	-3.510	1.00	20.72	C
ATOM	901	O	VAL	A	445	-5.107	3.002	-3.225	1.00	21.91	O
ATOM	902	N	SER	A	446	-5.184	5.244	-3.316	1.00	18.98	N
ATOM	903	CA	SER	A	446	-6.543	5.260	-2.734	1.00	19.98	C
ATOM	904	CB	SER	A	446	-6.988	6.704	-2.353	1.00	21.69	C
ATOM	905	OG	SER	A	446	-7.327	7.481	-3.468	1.00	24.84	O
ATOM	906	C	SER	A	446	-7.573	4.627	-3.662	1.00	20.82	C
ATOM	907	O	SER	A	446	-8.553	4.037	-3.187	1.00	21.15	O
ATOM	908	N	MET	A	447	-7.366	4.714	-4.974	1.00	19.01	N
ATOM	909	CA	MET	A	447	-8.294	4.078	-5.909	1.00	22.58	C
ATOM	910	CB	MET	A	447	-8.071	4.588	-7.347	1.00	23.29	C
ATOM	911	CG	MET	A	447	-8.540	6.039	-7.513	1.00	27.40	C
ATOM	912	SD	MET	A	447	-8.500	6.538	-9.288	1.00	29.46	S
ATOM	913	CE	MET	A	447	-6.769	6.928	-9.496	1.00	28.17	C
ATOM	914	C	MET	A	447	-8.133	2.558	-5.838	1.00	25.02	C
ATOM	915	O	MET	A	447	-9.114	1.821	-5.859	1.00	22.91	O

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ATOM    916  N    GLY A 448      -6.903   2.076  -5.729  1.00 20.29           N
ATOM    917  CA   GLY A 448      -6.712   0.644  -5.625  1.00 22.77           C
ATOM    918  C    GLY A 448      -7.337   0.135  -4.327  1.00 23.66           C
ATOM    919  O    GLY A 448      -7.963  -0.934  -4.331  1.00 24.13           O
ATOM    920  N    MET A 449      -7.192   0.892  -3.236  1.00 22.40           N
ATOM    921  CA   MET A 449      -7.756   0.450  -1.939  1.00 21.23           C
ATOM    922  CB   MET A 449      -7.139   1.232  -0.775  1.00 20.57           C
ATOM    923  CG   MET A 449      -5.611   1.012  -0.550  1.00 19.53           C
ATOM    924  SD   MET A 449      -5.170  -0.771  -0.382  1.00 25.09           S
ATOM    925  CE   MET A 449      -6.110  -1.175   1.087  1.00 26.33           C
ATOM    926  C    MET A 449      -9.282   0.566  -1.888  1.00 22.12           C
ATOM    927  O    MET A 449      -9.964  -0.236  -1.245  1.00 22.36           O
ATOM    928  N    LYS A 450      -9.832   1.554  -2.578  1.00 21.36           N
ATOM    929  CA   LYS A 450     -11.276   1.705  -2.642  1.00 22.17           C
ATOM    930  CB   LYS A 450     -11.616   2.949  -3.457  1.00 24.95           C
ATOM    931  CG   LYS A 450     -13.113   3.108  -3.668  1.00 34.59           C
ATOM    932  CD   LYS A 450     -13.388   4.170  -4.678  1.00 35.54           C
ATOM    933  CE   LYS A 450     -14.854   4.088  -5.081  1.00 43.28           C
ATOM    934  NZ   LYS A 450     -15.200   5.226  -5.962  1.00 51.23           N
ATOM    935  C    LYS A 450     -11.811   0.436  -3.328  1.00 20.54           C
ATOM    936  O    LYS A 450     -12.829  -0.138  -2.926  1.00 23.77           O
ATOM    937  N    TYR A 451     -11.093  -0.035  -4.339  1.00 22.16           N
ATOM    938  CA   TYR A 451     -11.490  -1.254  -5.053  1.00 25.84           C
ATOM    939  CB   TYR A 451     -10.606  -1.466  -6.295  1.00 30.33           C
ATOM    940  CG   TYR A 451     -10.851  -2.776  -7.036  1.00 26.97           C
ATOM    941  CD1  TYR A 451     -11.957  -2.942  -7.887  1.00 32.31           C
ATOM    942  CE1  TYR A 451     -12.156  -4.161  -8.577  1.00 35.26           C
ATOM    943  CD2  TYR A 451      -9.975  -3.841  -6.887  1.00 29.55           C
ATOM    944  CE2  TYR A 451     -10.171  -5.039  -7.538  1.00 38.20           C
ATOM    945  CZ   TYR A 451     -11.250  -5.202  -8.384  1.00 34.79           C
ATOM    946  OH   TYR A 451     -11.351  -6.416  -9.028  1.00 33.34           O
ATOM    947  C    TYR A 451     -11.413  -2.477  -4.156  1.00 25.12           C
ATOM    948  O    TYR A 451     -12.349  -3.279  -4.111  1.00 21.15           O
ATOM    949  N    LEU A 452     -10.317  -2.621  -3.411  1.00 23.09           N
ATOM    950  CA   LEU A 452     -10.190  -3.769  -2.528  1.00 22.43           C
ATOM    951  CB   LEU A 452      -8.812  -3.775  -1.805  1.00 24.62           C
ATOM    952  CG   LEU A 452      -7.633  -4.080  -2.723  1.00 29.88           C
ATOM    953  CD1  LEU A 452      -6.355  -3.885  -1.901  1.00 40.57           C
ATOM    954  CD2  LEU A 452      -7.706  -5.499  -3.261  1.00 37.63           C
ATOM    955  C    LEU A 452     -11.289  -3.770  -1.487  1.00 23.29           C
ATOM    956  O    LEU A 452     -11.835  -4.835  -1.160  1.00 24.20           O
ATOM    957  N    GLU A 453     -11.615  -2.586  -0.966  1.00 21.59           N
ATOM    958  CA   GLU A 453     -12.644  -2.465   0.044  1.00 23.71           C
ATOM    959  CB   GLU A 453     -12.707  -1.020   0.530  1.00 26.43           C
ATOM    960  CG   GLU A 453     -13.831  -0.730   1.519  1.00 27.65           C
ATOM    961  CD   GLU A 453     -13.831   0.727   1.990  1.00 34.87           C
ATOM    962  OE1  GLU A 453     -14.451   1.582   1.298  1.00 33.02           O
ATOM    963  OE2  GLU A 453     -13.200   1.012   3.042  1.00 30.22           O
ATOM    964  C    GLU A 453     -14.014  -2.901  -0.520  1.00 27.31           C
ATOM    965  O    GLU A 453     -14.763  -3.656   0.129  1.00 25.17           O
ATOM    966  N    GLU A 454     -14.348  -2.407  -1.706  1.00 22.10           N
ATOM    967  CA   GLU A 454     -15.640  -2.769  -2.310  1.00 25.66           C
ATOM    968  CB   GLU A 454     -15.871  -1.997  -3.619  1.00 31.24           C
ATOM    969  CG   GLU A 454     -14.964  -2.392  -4.754  1.00 42.57           C
ATOM    970  CD   GLU A 454     -15.261  -1.624  -6.046  1.00 58.39           C
ATOM    971  OE1  GLU A 454     -15.273  -0.363  -6.015  1.00 51.95           O
ATOM    972  OE2  GLU A 454     -15.472  -2.287  -7.094  1.00 58.17           O
ATOM    973  C    GLU A 454     -15.721  -4.263  -2.581  1.00 31.04           C
ATOM    974  O    GLU A 454     -16.810  -4.837  -2.583  1.00 30.48           O
ATOM    975  N    LYS A 455     -14.583  -4.915  -2.799  1.00 24.65           N
ATOM    976  CA   LYS A 455     -14.580  -6.358  -3.056  1.00 26.01           C
ATOM    977  CB   LYS A 455     -13.474  -6.742  -4.058  1.00 26.87           C
ATOM    978  CG   LYS A 455     -13.600  -6.047  -5.435  1.00 32.48           C
ATOM    979  CD   LYS A 455     -14.919  -6.413  -6.093  1.00 34.46           C
ATOM    980  CE   LYS A 455     -15.166  -5.643  -7.397  1.00 39.80           C
ATOM    981  NZ   LYS A 455     -16.498  -6.028  -7.995  1.00 35.47           N
ATOM    982  C    LYS A 455     -14.402  -7.158  -1.764  1.00 25.88           C
ATOM    983  O    LYS A 455     -14.205  -8.367  -1.799  1.00 33.28           O
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ATOM	984	N	ASN	A	456	-14.484	-6.474	-0.632	1.00	26.80	N
ATOM	985	CA	ASN	A	456	-14.348	-7.110	0.679	1.00	33.33	C
ATOM	986	CB	ASN	A	456	-15.537	-8.042	0.956	1.00	33.66	C
ATOM	987	CG	ASN	A	456	-16.833	-7.293	1.019	1.00	41.21	C
ATOM	988	OD1	ASN	A	456	-17.005	-6.397	1.847	1.00	38.41	O
ATOM	989	ND2	ASN	A	456	-17.763	-7.640	0.128	1.00	43.69	N
ATOM	990	C	ASN	A	456	-13.048	-7.865	0.932	1.00	32.96	C
ATOM	991	O	ASN	A	456	-13.065	-8.982	1.447	1.00	29.31	O
ATOM	992	N	PHE	A	457	-11.925	-7.265	0.539	1.00	25.61	N
ATOM	993	CA	PHE	A	457	-10.633	-7.871	0.827	1.00	23.17	C
ATOM	994	CB	PHE	A	457	-9.823	-8.104	-0.457	1.00	24.54	C
ATOM	995	CG	PHE	A	457	-10.302	-9.259	-1.274	1.00	27.01	C
ATOM	996	CD1	PHE	A	457	-11.141	-9.064	-2.372	1.00	38.40	C
ATOM	997	CD2	PHE	A	457	-9.912	-10.546	-0.952	1.00	30.92	C
ATOM	998	CE1	PHE	A	457	-11.573	-10.154	-3.131	1.00	40.99	C
ATOM	999	CE2	PHE	A	457	-10.338	-11.633	-1.702	1.00	39.35	C
ATOM	1000	CZ	PHE	A	457	-11.169	-11.435	-2.792	1.00	32.26	C
ATOM	1001	C	PHE	A	457	-9.876	-6.876	1.724	1.00	22.95	C
ATOM	1002	O	PHE	A	457	-10.006	-5.666	1.538	1.00	26.81	O
ATOM	1003	N	VAL	A	458	-9.095	-7.404	2.677	1.00	22.07	N
ATOM	1004	CA	VAL	A	458	-8.271	-6.587	3.574	1.00	18.40	C
ATOM	1005	CB	VAL	A	458	-8.476	-6.999	5.067	1.00	24.28	C
ATOM	1006	CG1	VAL	A	458	-7.490	-6.239	5.978	1.00	19.09	C
ATOM	1007	CG2	VAL	A	458	-9.885	-6.680	5.496	1.00	24.91	C
ATOM	1008	C	VAL	A	458	-6.811	-6.870	3.172	1.00	21.95	C
ATOM	1009	O	VAL	A	458	-6.412	-8.007	3.081	1.00	22.78	O
ATOM	1010	N	HIS	A	459	-6.017	-5.836	2.953	1.00	23.11	N
ATOM	1011	CA	HIS	A	459	-4.620	-6.058	2.514	1.00	22.90	C
ATOM	1012	CB	HIS	A	459	-4.106	-4.777	1.821	1.00	25.33	C
ATOM	1013	CG	HIS	A	459	-2.735	-4.915	1.233	1.00	27.05	C
ATOM	1014	CD2	HIS	A	459	-2.319	-4.984	-0.055	1.00	35.51	C
ATOM	1015	ND1	HIS	A	459	-1.598	-4.995	2.004	1.00	30.45	N
ATOM	1016	CE1	HIS	A	459	-0.539	-5.097	1.218	1.00	30.89	C
ATOM	1017	NE2	HIS	A	459	-0.950	-5.091	-0.037	1.00	27.20	N
ATOM	1018	C	HIS	A	459	-3.726	-6.406	3.702	1.00	22.15	C
ATOM	1019	O	HIS	A	459	-2.926	-7.373	3.669	1.00	26.50	O
ATOM	1020	N	ARG	A	460	-3.870	-5.592	4.743	1.00	22.61	N
ATOM	1021	CA	ARG	A	460	-3.160	-5.697	6.007	1.00	21.98	C
ATOM	1022	CB	ARG	A	460	-3.202	-7.138	6.526	1.00	27.77	C
ATOM	1023	CG	ARG	A	460	-2.704	-7.226	7.957	1.00	39.24	C
ATOM	1024	CD	ARG	A	460	-2.722	-8.632	8.504	1.00	31.08	C
ATOM	1025	NE	ARG	A	460	-1.706	-8.745	9.539	1.00	33.21	N
ATOM	1026	CZ	ARG	A	460	-1.459	-9.857	10.236	1.00	39.79	C
ATOM	1027	NH1	ARG	A	460	-2.161	-10.955	10.014	1.00	32.10	N
ATOM	1028	NH2	ARG	A	460	-0.492	-9.866	11.146	1.00	40.69	N
ATOM	1029	C	ARG	A	460	-1.706	-5.211	6.022	1.00	28.94	C
ATOM	1030	O	ARG	A	460	-1.177	-4.874	7.079	1.00	36.64	O
ATOM	1031	N	ASP	A	461	-1.072	-5.145	4.861	1.00	24.64	N
ATOM	1032	CA	ASP	A	461	0.325	-4.733	4.836	1.00	26.58	C
ATOM	1033	CB	ASP	A	461	1.172	-5.943	4.374	1.00	27.03	C
ATOM	1034	CG	ASP	A	461	2.667	-5.827	4.743	1.00	38.59	C
ATOM	1035	OD1	ASP	A	461	3.050	-4.953	5.551	1.00	48.65	O
ATOM	1036	OD2	ASP	A	461	3.468	-6.646	4.224	1.00	49.76	O
ATOM	1037	C	ASP	A	461	0.521	-3.500	3.932	1.00	27.57	C
ATOM	1038	O	ASP	A	461	1.524	-3.370	3.237	1.00	26.49	O
ATOM	1039	N	LEU	A	462	-0.429	-2.572	3.956	1.00	22.27	N
ATOM	1040	CA	LEU	A	462	-0.278	-1.380	3.139	1.00	21.53	C
ATOM	1041	CB	LEU	A	462	-1.636	-0.666	2.987	1.00	22.43	C
ATOM	1042	CG	LEU	A	462	-1.648	0.602	2.128	1.00	30.85	C
ATOM	1043	CD1	LEU	A	462	-1.215	0.224	0.715	1.00	29.37	C
ATOM	1044	CD2	LEU	A	462	-3.042	1.270	2.133	1.00	27.57	C
ATOM	1045	C	LEU	A	462	0.779	-0.477	3.804	1.00	22.66	C
ATOM	1046	O	LEU	A	462	0.671	-0.125	4.950	1.00	26.45	O
ATOM	1047	N	ALA	A	463	1.832	-0.159	3.063	1.00	21.02	N
ATOM	1048	CA	ALA	A	463	2.926	0.688	3.572	1.00	19.38	C
ATOM	1049	CB	ALA	A	463	3.865	-0.138	4.481	1.00	20.15	C
ATOM	1050	C	ALA	A	463	3.669	1.169	2.323	1.00	17.38	C
ATOM	1051	O	ALA	A	463	3.586	0.534	1.274	1.00	21.49	O

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ATOM	1052	N	ALA	A	464	4.383	2.277	2.438	1.00	20.81	N
ATOM	1053	CA	ALA	A	464	5.062	2.797	1.271	1.00	22.24	C
ATOM	1054	CB	ALA	A	464	5.810	4.094	1.651	1.00	19.74	C
ATOM	1055	C	ALA	A	464	6.005	1.777	0.641	1.00	23.62	C
ATOM	1056	O	ALA	A	464	6.180	1.782	-0.571	1.00	22.85	O
ATOM	1057	N	ARG	A	465	6.611	0.915	1.457	1.00	23.55	N
ATOM	1058	CA	ARG	A	465	7.528	-0.112	0.962	1.00	22.78	C
ATOM	1059	CB	ARG	A	465	8.203	-0.852	2.133	1.00	26.22	C
ATOM	1060	CG	ARG	A	465	7.254	-1.662	3.026	1.00	22.40	C
ATOM	1061	CD	ARG	A	465	7.980	-2.238	4.272	1.00	27.73	C
ATOM	1062	NE	ARG	A	465	7.030	-2.873	5.180	1.00	32.59	N
ATOM	1063	CZ	ARG	A	465	6.337	-2.232	6.126	1.00	41.47	C
ATOM	1064	NH1	ARG	A	465	6.491	-0.928	6.320	1.00	34.18	N
ATOM	1065	NH2	ARG	A	465	5.441	-2.887	6.841	1.00	40.07	N
ATOM	1066	C	ARG	A	465	6.814	-1.136	0.084	1.00	24.95	C
ATOM	1067	O	ARG	A	465	7.461	-1.867	-0.673	1.00	25.58	O
ATOM	1068	N	ASN	A	466	5.484	-1.203	0.199	1.00	24.98	N
ATOM	1069	CA	ASN	A	466	4.715	-2.149	-0.603	1.00	23.15	C
ATOM	1070	CB	ASN	A	466	3.785	-2.982	0.276	1.00	20.54	C
ATOM	1071	CG	ASN	A	466	4.537	-3.987	1.118	1.00	29.73	C
ATOM	1072	OD1	ASN	A	466	5.600	-4.469	0.710	1.00	26.55	O
ATOM	1073	ND2	ASN	A	466	4.000	-4.310	2.302	1.00	25.54	N
ATOM	1074	C	ASN	A	466	3.947	-1.509	-1.752	1.00	23.75	C
ATOM	1075	O	ASN	A	466	3.185	-2.171	-2.442	1.00	24.79	O
ATOM	1076	N	VAL	A	467	4.170	-0.220	-1.959	1.00	21.31	N
ATOM	1077	CA	VAL	A	467	3.561	0.462	-3.086	1.00	19.34	C
ATOM	1078	CB	VAL	A	467	3.127	1.872	-2.699	1.00	21.47	C
ATOM	1079	CG1	VAL	A	467	2.736	2.647	-3.979	1.00	22.29	C
ATOM	1080	CG2	VAL	A	467	1.957	1.792	-1.696	1.00	19.95	C
ATOM	1081	C	VAL	A	467	4.733	0.538	-4.076	1.00	22.01	C
ATOM	1082	O	VAL	A	467	5.817	1.025	-3.721	1.00	22.82	O
ATOM	1083	N	LEU	A	468	4.524	0.036	-5.290	1.00	21.63	N
ATOM	1084	CA	LEU	A	468	5.601	0.021	-6.286	1.00	25.97	C
ATOM	1085	CB	LEU	A	468	5.828	-1.399	-6.801	1.00	21.35	C
ATOM	1086	CG	LEU	A	468	6.073	-2.498	-5.767	1.00	25.31	C
ATOM	1087	CD1	LEU	A	468	5.995	-3.859	-6.430	1.00	25.16	C
ATOM	1088	CD2	LEU	A	468	7.434	-2.267	-5.110	1.00	27.20	C
ATOM	1089	C	LEU	A	468	5.285	0.920	-7.465	1.00	29.27	C
ATOM	1090	O	LEU	A	468	4.143	1.006	-7.884	1.00	26.29	O
ATOM	1091	N	LEU	A	469	6.311	1.554	-8.035	1.00	24.41	N
ATOM	1092	CA	LEU	A	469	6.063	2.440	-9.156	1.00	25.24	C
ATOM	1093	CB	LEU	A	469	6.886	3.714	-8.973	1.00	28.20	C
ATOM	1094	CG	LEU	A	469	6.583	4.441	-7.661	1.00	40.39	C
ATOM	1095	CD1	LEU	A	469	7.566	5.547	-7.471	1.00	42.75	C
ATOM	1096	CD2	LEU	A	469	5.180	5.007	-7.681	1.00	36.92	C
ATOM	1097	C	LEU	A	469	6.356	1.844	-10.518	1.00	25.99	C
ATOM	1098	O	LEU	A	469	7.411	1.237	-10.729	1.00	27.91	O
ATOM	1099	N	VAL	A	470	5.416	1.985	-11.445	1.00	27.37	N
ATOM	1100	CA	VAL	A	470	5.662	1.526	-12.795	1.00	27.70	C
ATOM	1101	CB	VAL	A	470	4.369	1.352	-13.589	1.00	30.57	C
ATOM	1102	CG1	VAL	A	470	4.693	1.012	-15.042	1.00	35.99	C
ATOM	1103	CG2	VAL	A	470	3.536	0.219	-12.963	1.00	28.74	C
ATOM	1104	C	VAL	A	470	6.517	2.663	-13.384	1.00	32.73	C
ATOM	1105	O	VAL	A	470	7.467	2.415	-14.137	1.00	35.56	O
ATOM	1106	N	ASN	A	471	6.172	3.895	-13.012	1.00	30.05	N
ATOM	1107	CA	ASN	A	471	6.889	5.122	-13.415	1.00	35.49	C
ATOM	1108	CB	ASN	A	471	6.441	5.610	-14.805	1.00	38.79	C
ATOM	1109	CG	ASN	A	471	4.941	5.766	-14.912	1.00	38.59	C
ATOM	1110	OD1	ASN	A	471	4.246	4.841	-15.320	1.00	61.19	O
ATOM	1111	ND2	ASN	A	471	4.432	6.917	-14.518	1.00	37.18	N
ATOM	1112	C	ASN	A	471	6.561	6.186	-12.366	1.00	34.10	C
ATOM	1113	O	ASN	A	471	5.766	5.925	-11.458	1.00	31.54	O
ATOM	1114	N	ARG	A	472	7.144	7.383	-12.468	1.00	31.44	N
ATOM	1115	CA	ARG	A	472	6.889	8.423	-11.467	1.00	34.23	C
ATOM	1116	CB	ARG	A	472	7.812	9.628	-11.699	1.00	36.29	C
ATOM	1117	CG	ARG	A	472	7.539	10.352	-13.002	1.00	38.64	C
ATOM	1118	CD	ARG	A	472	8.440	11.577	-13.126	1.00	42.01	C
ATOM	1119	NE	ARG	A	472	7.960	12.686	-12.310	1.00	42.62	N

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ATOM	1120	CZ	ARG	A	472	8.611	13.835	-12.142	1.00	49.56	C
ATOM	1121	NH1	ARG	A	472	9.789	14.036	-12.734	1.00	41.21	N
ATOM	1122	NH2	ARG	A	472	8.082	14.791	-11.395	1.00	45.67	N
ATOM	1123	C	ARG	A	472	5.442	8.907	-11.393	1.00	23.39	C
ATOM	1124	O	ARG	A	472	5.087	9.644	-10.491	1.00	29.27	O
ATOM	1125	N	HIS	A	473	4.621	8.504	-12.357	1.00	26.03	N
ATOM	1126	CA	HIS	A	473	3.234	8.911	-12.392	1.00	32.63	C
ATOM	1127	CB	HIS	A	473	2.947	9.729	-13.680	1.00	27.76	C
ATOM	1128	CG	HIS	A	473	3.693	11.026	-13.743	1.00	31.49	C
ATOM	1129	CD2	HIS	A	473	4.728	11.426	-14.522	1.00	40.44	C
ATOM	1130	ND1	HIS	A	473	3.462	12.056	-12.858	1.00	33.49	N
ATOM	1131	CE1	HIS	A	473	4.327	13.031	-13.082	1.00	42.59	C
ATOM	1132	NE2	HIS	A	473	5.108	12.673	-14.086	1.00	41.30	N
ATOM	1133	C	HIS	A	473	2.296	7.710	-12.329	1.00	28.13	C
ATOM	1134	O	HIS	A	473	1.105	7.842	-12.651	1.00	25.55	O
ATOM	1135	N	TYR	A	474	2.813	6.547	-11.928	1.00	26.97	N
ATOM	1136	CA	TYR	A	474	1.957	5.357	-11.889	1.00	29.51	C
ATOM	1137	CB	TYR	A	474	1.991	4.652	-13.250	1.00	26.22	C
ATOM	1138	CG	TYR	A	474	0.982	3.515	-13.472	1.00	30.97	C
ATOM	1139	CD1	TYR	A	474	-0.077	3.274	-12.582	1.00	28.77	C
ATOM	1140	CE1	TYR	A	474	-1.001	2.218	-12.823	1.00	31.08	C
ATOM	1141	CD2	TYR	A	474	1.091	2.689	-14.596	1.00	33.81	C
ATOM	1142	CE2	TYR	A	474	0.191	1.658	-14.838	1.00	34.98	C
ATOM	1143	CZ	TYR	A	474	-0.853	1.418	-13.960	1.00	33.21	C
ATOM	1144	OH	TYR	A	474	-1.723	0.375	-14.256	1.00	31.45	O
ATOM	1145	C	TYR	A	474	2.358	4.376	-10.789	1.00	25.47	C
ATOM	1146	O	TYR	A	474	3.336	3.636	-10.932	1.00	28.97	O
ATOM	1147	N	ALA	A	475	1.571	4.374	-9.710	1.00	22.78	N
ATOM	1148	CA	ALA	A	475	1.837	3.495	-8.577	1.00	26.62	C
ATOM	1149	CB	ALA	A	475	1.696	4.297	-7.265	1.00	27.18	C
ATOM	1150	C	ALA	A	475	0.897	2.280	-8.553	1.00	28.20	C
ATOM	1151	O	ALA	A	475	-0.234	2.341	-9.045	1.00	25.92	O
ATOM	1152	N	LYS	A	476	1.380	1.169	-7.990	1.00	24.41	N
ATOM	1153	CA	LYS	A	476	0.569	-0.039	-7.855	1.00	23.63	C
ATOM	1154	CB	LYS	A	476	0.957	-1.092	-8.912	1.00	26.51	C
ATOM	1155	CG	LYS	A	476	0.418	-0.795	-10.305	1.00	27.53	C
ATOM	1156	CD	LYS	A	476	0.985	-1.811	-11.310	1.00	32.34	C
ATOM	1157	CE	LYS	A	476	0.273	-1.748	-12.657	1.00	36.56	C
ATOM	1158	NZ	LYS	A	476	-0.989	-2.542	-12.605	1.00	37.90	N
ATOM	1159	C	LYS	A	476	0.772	-0.657	-6.477	1.00	25.52	C
ATOM	1160	O	LYS	A	476	1.898	-0.684	-5.956	1.00	25.22	O
ATOM	1161	N	ILE	A	477	-0.309	-1.172	-5.896	1.00	22.11	N
ATOM	1162	CA	ILE	A	477	-0.214	-1.800	-4.580	1.00	24.01	C
ATOM	1163	CB	ILE	A	477	-1.577	-1.846	-3.915	1.00	21.78	C
ATOM	1164	CG2	ILE	A	477	-1.499	-2.642	-2.596	1.00	25.26	C
ATOM	1165	CG1	ILE	A	477	-2.081	-0.417	-3.708	1.00	20.73	C
ATOM	1166	CD1	ILE	A	477	-3.578	-0.332	-3.534	1.00	22.58	C
ATOM	1167	C	ILE	A	477	0.267	-3.223	-4.766	1.00	24.46	C
ATOM	1168	O	ILE	A	477	-0.216	-3.919	-5.654	1.00	22.86	O
ATOM	1169	N	SER	A	478	1.214	-3.666	-3.932	1.00	22.32	N
ATOM	1170	CA	SER	A	478	1.691	-5.039	-4.071	1.00	22.20	C
ATOM	1171	CB	SER	A	478	3.097	-5.049	-4.649	1.00	28.05	C
ATOM	1172	OG	SER	A	478	3.965	-4.509	-3.674	1.00	38.71	O
ATOM	1173	C	SER	A	478	1.723	-5.787	-2.738	1.00	26.29	C
ATOM	1174	O	SER	A	478	1.311	-5.261	-1.697	1.00	25.87	O
ATOM	1175	N	ASP	A	479	2.247	-7.010	-2.810	1.00	23.81	N
ATOM	1176	CA	ASP	A	479	2.394	-7.959	-1.690	1.00	25.45	C
ATOM	1177	CB	ASP	A	479	3.465	-7.519	-0.666	1.00	24.64	C
ATOM	1178	CG	ASP	A	479	3.850	-8.676	0.288	1.00	35.61	C
ATOM	1179	OD1	ASP	A	479	3.141	-9.710	0.289	1.00	30.47	O
ATOM	1180	OD2	ASP	A	479	4.860	-8.567	1.018	1.00	31.61	O
ATOM	1181	C	ASP	A	479	1.099	-8.294	-0.952	1.00	21.75	C
ATOM	1182	O	ASP	A	479	0.819	-7.751	0.144	1.00	21.47	O
ATOM	1183	N	PHE	A	480	0.359	-9.246	-1.524	1.00	24.40	N
ATOM	1184	CA	PHE	A	480	-0.905	-9.719	-0.946	1.00	27.55	C
ATOM	1185	CB	PHE	A	480	-1.910	-9.973	-2.077	1.00	22.84	C
ATOM	1186	CG	PHE	A	480	-2.335	-8.709	-2.776	1.00	25.54	C
ATOM	1187	CD1	PHE	A	480	-3.472	-7.999	-2.373	1.00	37.22	C

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ATOM   1188  CD2 PHE A 480     -1.531  -8.165  -3.774  1.00 29.75           C
ATOM   1189  CE1 PHE A 480     -3.788  -6.767  -2.950  1.00 36.53           C
ATOM   1190  CE2 PHE A 480     -1.841  -6.925  -4.351  1.00 31.15           C
ATOM   1191  CZ  PHE A 480     -2.956  -6.229  -3.945  1.00 30.92           C
ATOM   1192  C   PHE A 480     -0.734 -10.978  -0.070  1.00 22.25           C
ATOM   1193  O   PHE A 480     -1.693 -11.697   0.201  1.00 28.80           O
ATOM   1194  N   GLY A 481      0.494 -11.200   0.395  1.00 26.68           N
ATOM   1195  CA  GLY A 481      0.808 -12.354   1.234  1.00 25.28           C
ATOM   1196  C   GLY A 481      0.041 -12.422   2.553  1.00 29.85           C
ATOM   1197  O   GLY A 481     -0.094 -13.489   3.125  1.00 28.84           O
ATOM   1198  N   LEU A 482     -0.455 -11.293   3.049  1.00 21.56           N
ATOM   1199  CA  LEU A 482     -1.217 -11.299   4.316  1.00 23.95           C
ATOM   1200  CB  LEU A 482     -0.608 -10.287   5.304  1.00 25.94           C
ATOM   1201  CG  LEU A 482      0.789 -10.660   5.792  1.00 31.12           C
ATOM   1202  CD1 LEU A 482      1.418  -9.482   6.554  1.00 34.67           C
ATOM   1203  CD2 LEU A 482      0.680 -11.884   6.675  1.00 35.08           C
ATOM   1204  C   LEU A 482     -2.667 -10.925   4.097  1.00 21.10           C
ATOM   1205  O   LEU A 482     -3.441 -10.766   5.050  1.00 26.73           O
ATOM   1206  N   SER A 483     -3.050 -10.794   2.837  1.00 21.83           N
ATOM   1207  CA  SER A 483     -4.409 -10.375   2.518  1.00 17.76           C
ATOM   1208  CB  SER A 483     -4.465  -9.958   1.042  1.00 22.28           C
ATOM   1209  OG  SER A 483     -3.595  -8.851   0.860  1.00 29.25           O
ATOM   1210  C   SER A 483     -5.440 -11.475   2.785  1.00 21.06           C
ATOM   1211  O   SER A 483     -5.128 -12.645   2.739  1.00 24.20           O
ATOM   1212  N   LYS A 484     -6.681 -11.071   3.034  1.00 20.71           N
ATOM   1213  CA  LYS A 484     -7.738 -12.041   3.291  1.00 21.00           C
ATOM   1214  CB  LYS A 484     -7.862 -12.318   4.791  1.00 24.78           C
ATOM   1215  CG  LYS A 484     -6.650 -13.105   5.362  1.00 38.83           C
ATOM   1216  CD  LYS A 484     -6.770 -13.393   6.859  1.00 45.27           C
ATOM   1217  CE  LYS A 484     -5.677 -14.378   7.302  1.00 43.33           C
ATOM   1218  NZ  LYS A 484     -4.326 -14.049   6.778  1.00 56.25           N
ATOM   1219  C   LYS A 484     -9.076 -11.545   2.768  1.00 25.54           C
ATOM   1220  O   LYS A 484     -9.320 -10.348   2.677  1.00 26.31           O
ATOM   1221  N   ALA A 485     -9.941 -12.491   2.434  1.00 23.65           N
ATOM   1222  CA  ALA A 485    -11.280 -12.138   1.974  1.00 22.67           C
ATOM   1223  CB  ALA A 485    -11.814 -13.210   0.995  1.00 31.69           C
ATOM   1224  C   ALA A 485    -12.144 -12.086   3.249  1.00 31.19           C
ATOM   1225  O   ALA A 485    -12.006 -12.931   4.136  1.00 29.37           O
ATOM   1226  N   LEU A 486    -12.995 -11.073   3.349  1.00 23.82           N
ATOM   1227  CA  LEU A 486    -13.873 -10.926   4.518  1.00 20.69           C
ATOM   1228  CB  LEU A 486    -14.113  -9.435   4.825  1.00 28.46           C
ATOM   1229  CG  LEU A 486    -13.031  -8.604   5.532  1.00 31.01           C
ATOM   1230  CD1 LEU A 486    -13.418  -7.137   5.591  1.00 36.09           C
ATOM   1231  CD2 LEU A 486    -12.840  -9.129   6.923  1.00 37.43           C
ATOM   1232  C   LEU A 486    -15.239 -11.583   4.288  1.00 31.06           C
ATOM   1233  O   LEU A 486    -15.911 -11.953   5.235  1.00 33.37           O
ATOM   1234  N   GLY A 487    -15.651 -11.715   3.031  1.00 28.59           N
ATOM   1235  CA  GLY A 487    -16.955 -12.284   2.753  1.00 33.58           C
ATOM   1236  C   GLY A 487    -18.031 -11.345   3.283  1.00 38.11           C
ATOM   1237  O   GLY A 487    -17.980 -10.144   3.077  1.00 36.30           O
ATOM   1238  N   ALA A 488    -18.987 -11.910   4.004  1.00 38.66           N
ATOM   1239  CA  ALA A 488    -20.092 -11.130   4.556  1.00 40.22           C
ATOM   1240  CB  ALA A 488    -21.287 -12.045   4.812  1.00 46.29           C
ATOM   1241  C   ALA A 488    -19.733 -10.388   5.843  1.00 40.58           C
ATOM   1242  O   ALA A 488    -20.483  -9.532   6.295  1.00 40.10           O
ATOM   1243  N   ASP A 489    -18.578 -10.699   6.422  1.00 36.35           N
ATOM   1244  CA  ASP A 489    -18.160 -10.041   7.672  1.00 35.41           C
ATOM   1245  CB  ASP A 489    -17.192 -10.955   8.431  1.00 37.29           C
ATOM   1246  CG  ASP A 489    -17.782 -12.314   8.686  1.00 49.00           C
ATOM   1247  OD1 ASP A 489    -19.013 -12.383   8.909  1.00 49.08           O
ATOM   1248  OD2 ASP A 489    -17.018 -13.305   8.680  1.00 50.85           O
ATOM   1249  C   ASP A 489    -17.508  -8.676   7.484  1.00 30.55           C
ATOM   1250  O   ASP A 489    -16.974  -8.388   6.427  1.00 32.36           O
ATOM   1251  N   ASP A 490    -17.538  -7.845   8.529  1.00 28.02           N
ATOM   1252  CA  ASP A 490    -16.923  -6.527   8.441  1.00 31.41           C
ATOM   1253  CB  ASP A 490    -17.768  -5.486   9.178  1.00 38.68           C
ATOM   1254  CG  ASP A 490    -17.934  -5.812  10.630  1.00 48.46           C
ATOM   1255  OD1 ASP A 490    -18.996  -5.471  11.213  1.00 57.52           O
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ATOM	1256	OD2	ASP	A	490	-16.999	-6.397	11.198	1.00	54.69	O
ATOM	1257	C	ASP	A	490	-15.492	-6.523	8.983	1.00	26.85	C
ATOM	1258	O	ASP	A	490	-14.799	-5.512	8.906	1.00	24.78	O
ATOM	1259	N	SER	A	491	-15.046	-7.652	9.521	1.00	23.91	N
ATOM	1260	CA	SER	A	491	-13.666	-7.760	10.031	1.00	22.38	C
ATOM	1261	CB	SER	A	491	-13.522	-6.993	11.336	1.00	29.00	C
ATOM	1262	OG	SER	A	491	-14.280	-7.634	12.371	1.00	32.97	O
ATOM	1263	C	SER	A	491	-13.333	-9.202	10.309	1.00	29.41	C
ATOM	1264	O	SER	A	491	-14.204	-10.076	10.200	1.00	25.81	O
ATOM	1265	N	TYR	A	492	-12.068	-9.462	10.640	1.00	23.00	N
ATOM	1266	CA	TYR	A	492	-11.679	-10.788	11.033	1.00	26.00	C
ATOM	1267	CB	TYR	A	492	-11.165	-11.647	9.858	1.00	26.94	C
ATOM	1268	CG	TYR	A	492	-9.811	-11.265	9.328	1.00	26.14	C
ATOM	1269	CD1	TYR	A	492	-8.639	-11.830	9.855	1.00	24.16	C
ATOM	1270	CE1	TYR	A	492	-7.378	-11.414	9.419	1.00	28.54	C
ATOM	1271	CD2	TYR	A	492	-9.693	-10.285	8.348	1.00	25.38	C
ATOM	1272	CE2	TYR	A	492	-8.424	-9.859	7.902	1.00	23.56	C
ATOM	1273	CZ	TYR	A	492	-7.282	-10.428	8.447	1.00	26.57	C
ATOM	1274	OH	TYR	A	492	-6.040	-9.993	8.045	1.00	24.90	O
ATOM	1275	C	TYR	A	492	-10.630	-10.613	12.122	1.00	23.17	C
ATOM	1276	O	TYR	A	492	-10.082	-9.521	12.308	1.00	22.18	O
ATOM	1277	N	TYR	A	493	-10.404	-11.690	12.865	1.00	21.40	N
ATOM	1278	CA	TYR	A	493	-9.406	-11.705	13.943	1.00	18.61	C
ATOM	1279	CB	TYR	A	493	-10.015	-12.168	15.262	1.00	23.77	C
ATOM	1280	CG	TYR	A	493	-10.965	-11.174	15.837	1.00	24.82	C
ATOM	1281	CD1	TYR	A	493	-12.229	-11.002	15.282	1.00	26.28	C
ATOM	1282	CE1	TYR	A	493	-13.105	-10.061	15.789	1.00	33.92	C
ATOM	1283	CD2	TYR	A	493	-10.598	-10.375	16.921	1.00	24.00	C
ATOM	1284	CE2	TYR	A	493	-11.468	-9.431	17.439	1.00	29.62	C
ATOM	1285	CZ	TYR	A	493	-12.719	-9.284	16.868	1.00	33.02	C
ATOM	1286	OH	TYR	A	493	-13.592	-8.384	17.410	1.00	32.06	O
ATOM	1287	C	TYR	A	493	-8.394	-12.708	13.459	1.00	19.01	C
ATOM	1288	O	TYR	A	493	-8.749	-13.842	13.091	1.00	22.83	O
ATOM	1289	N	THR	A	494	-7.141	-12.272	13.400	1.00	26.38	N
ATOM	1290	CA	THR	A	494	-6.077	-13.079	12.834	1.00	32.64	C
ATOM	1291	CB	THR	A	494	-5.029	-12.172	12.119	1.00	31.23	C
ATOM	1292	OG1	THR	A	494	-4.099	-12.987	11.401	1.00	41.68	O
ATOM	1293	CG2	THR	A	494	-4.270	-11.355	13.123	1.00	33.57	C
ATOM	1294	C	THR	A	494	-5.332	-13.934	13.830	1.00	34.49	C
ATOM	1295	O	THR	A	494	-5.210	-13.605	15.005	1.00	28.24	O
ATOM	1296	N	ALA	A	495	-4.747	-15.006	13.322	1.00	44.02	N
ATOM	1297	CA	ALA	A	495	-3.959	-15.870	14.166	1.00	49.59	C
ATOM	1298	CB	ALA	A	495	-3.887	-17.248	13.552	1.00	46.73	C
ATOM	1299	C	ALA	A	495	-2.562	-15.276	14.307	1.00	50.58	C
ATOM	1300	O	ALA	A	495	-2.108	-14.536	13.439	1.00	49.05	O
ATOM	1301	N	ARG	A	496	-1.899	-15.593	15.409	1.00	54.28	N
ATOM	1302	CA	ARG	A	496	-0.552	-15.110	15.668	1.00	58.65	C
ATOM	1303	CB	ARG	A	496	-0.261	-15.109	17.173	1.00	60.21	C
ATOM	1304	CG	ARG	A	496	0.432	-13.854	17.698	1.00	65.46	C
ATOM	1305	CD	ARG	A	496	1.644	-13.487	16.885	1.00	66.41	C
ATOM	1306	NE	ARG	A	496	2.227	-12.233	17.353	1.00	67.01	N
ATOM	1307	CZ	ARG	A	496	3.254	-11.624	16.771	1.00	70.08	C
ATOM	1308	NH1	ARG	A	496	3.816	-12.156	15.690	1.00	71.57	N
ATOM	1309	NH2	ARG	A	496	3.722	-10.486	17.268	1.00	67.36	N
ATOM	1310	C	ARG	A	496	0.441	-16.048	14.971	1.00	60.54	C
ATOM	1311	O	ARG	A	496	0.365	-17.270	15.112	1.00	59.09	O
ATOM	1312	N	SER	A	497	1.362	-15.475	14.209	1.00	58.17	N
ATOM	1313	CA	SER	A	497	2.370	-16.275	13.523	1.00	60.35	C
ATOM	1314	CB	SER	A	497	2.276	-16.074	12.010	1.00	60.39	C
ATOM	1315	OG	SER	A	497	2.664	-14.760	11.653	1.00	64.92	O
ATOM	1316	C	SER	A	497	3.736	-15.821	14.016	1.00	60.92	C
ATOM	1317	O	SER	A	497	3.836	-14.890	14.817	1.00	58.88	O
ATOM	1318	N	ALA	A	498	4.781	-16.480	13.531	1.00	63.41	N
ATOM	1319	CA	ALA	A	498	6.146	-16.143	13.911	1.00	61.88	C
ATOM	1320	CB	ALA	A	498	7.102	-17.263	13.482	1.00	59.84	C
ATOM	1321	C	ALA	A	498	6.556	-14.827	13.254	1.00	60.58	C
ATOM	1322	O	ALA	A	498	6.132	-14.515	12.138	1.00	60.40	O
ATOM	1323	N	GLY	A	499	7.381	-14.057	13.950	1.00	60.46	N

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ATOM   1324  CA  GLY A 499     7.833 -12.798  13.393  1.00 63.38          C
ATOM   1325  C   GLY A 499     7.226 -11.608  14.100  1.00 61.34          C
ATOM   1326  O   GLY A 499     6.240 -11.741  14.827  1.00 64.30          O
ATOM   1327  N   LYS A 500     7.817 -10.440  13.886  1.00 60.00          N
ATOM   1328  CA  LYS A 500     7.338  -9.216  14.511  1.00 56.90          C
ATOM   1329  CB  LYS A 500     8.502  -8.246  14.717  1.00 60.17          C
ATOM   1330  CG  LYS A 500     9.535  -8.705  15.729  1.00 63.00          C
ATOM   1331  CD  LYS A 500     8.991  -8.599  17.148  1.00 67.02          C
ATOM   1332  CE  LYS A 500    10.049  -8.992  18.174  1.00 65.56          C
ATOM   1333  NZ  LYS A 500     9.537  -8.897  19.573  1.00 68.82          N
ATOM   1334  C   LYS A 500     6.272  -8.539  13.654  1.00 51.76          C
ATOM   1335  O   LYS A 500     6.271  -8.656  12.434  1.00 48.14          O
ATOM   1336  N   TRP A 501     5.363  -7.829  14.311  1.00 47.51          N
ATOM   1337  CA  TRP A 501     4.307  -7.104  13.602  1.00 46.32          C
ATOM   1338  CB  TRP A 501     3.028  -7.109  14.441  1.00 41.88          C
ATOM   1339  CG  TRP A 501     2.225  -8.356  14.335  1.00 37.72          C
ATOM   1340  CD2 TRP A 501     0.855  -8.518  14.721  1.00 36.73          C
ATOM   1341  CE2 TRP A 501     0.471  -9.832  14.363  1.00 39.69          C
ATOM   1342  CE3 TRP A 501    -0.089  -7.679  15.334  1.00 38.48          C
ATOM   1343  CD1 TRP A 501     2.613  -9.547  13.789  1.00 42.00          C
ATOM   1344  NE1 TRP A 501     1.562 -10.441  13.797  1.00 38.68          N
ATOM   1345  CZ2 TRP A 501    -0.821 -10.325  14.593  1.00 35.30          C
ATOM   1346  CZ3 TRP A 501    -1.379  -8.176  15.565  1.00 32.86          C
ATOM   1347  CH2 TRP A 501    -1.726  -9.483  15.192  1.00 35.05          C
ATOM   1348  C   TRP A 501     4.765  -5.658  13.385  1.00 39.20          C
ATOM   1349  O   TRP A 501     5.361  -5.063  14.279  1.00 42.54          O
ATOM   1350  N   PRO A 502     4.500  -5.079  12.197  1.00 36.57          N
ATOM   1351  CD  PRO A 502     3.828  -5.725  11.050  1.00 35.66          C
ATOM   1352  CA  PRO A 502     4.885  -3.689  11.876  1.00 38.88          C
ATOM   1353  CB  PRO A 502     4.721  -3.623  10.359  1.00 37.46          C
ATOM   1354  CG  PRO A 502     3.547  -4.559  10.117  1.00 42.86          C
ATOM   1355  C   PRO A 502     3.908  -2.772  12.604  1.00 36.51          C
ATOM   1356  O   PRO A 502     3.018  -2.152  11.988  1.00 28.01          O
ATOM   1357  N   LEU A 503     4.079  -2.706  13.921  1.00 29.24          N
ATOM   1358  CA  LEU A 503     3.185  -1.931  14.780  1.00 29.71          C
ATOM   1359  CB  LEU A 503     3.701  -1.950  16.227  1.00 36.06          C
ATOM   1360  CG  LEU A 503     3.999  -3.328  16.817  1.00 39.54          C
ATOM   1361  CD1 LEU A 503     4.596  -3.172  18.215  1.00 48.04          C
ATOM   1362  CD2 LEU A 503     2.727  -4.145  16.872  1.00 43.63          C
ATOM   1363  C   LEU A 503     2.962  -0.489  14.364  1.00 25.89          C
ATOM   1364  O   LEU A 503     1.875   0.057  14.580  1.00 24.95          O
ATOM   1365  N   LYS A 504     3.979   0.132  13.766  1.00 24.94          N
ATOM   1366  CA  LYS A 504     3.860   1.527  13.379  1.00 25.26          C
ATOM   1367  CB  LYS A 504     5.223   2.090  12.978  1.00 28.02          C
ATOM   1368  CG  LYS A 504     6.170   2.228  14.194  1.00 31.43          C
ATOM   1369  CD  LYS A 504     7.500   2.881  13.813  1.00 31.17          C
ATOM   1370  CE  LYS A 504     8.447   2.979  15.011  1.00 36.32          C
ATOM   1371  NZ  LYS A 504     9.635   3.805  14.649  1.00 38.54          N
ATOM   1372  C   LYS A 504     2.846   1.772  12.264  1.00 26.30          C
ATOM   1373  O   LYS A 504     2.453   2.892  12.040  1.00 22.29          O
ATOM   1374  N   TRP A 505     2.430   0.719  11.581  1.00 22.68          N
ATOM   1375  CA  TRP A 505     1.437   0.866  10.515  1.00 18.95          C
ATOM   1376  CB  TRP A 505     1.890   0.096   9.275  1.00 25.33          C
ATOM   1377  CG  TRP A 505     2.892   0.834   8.461  1.00 25.92          C
ATOM   1378  CD2 TRP A 505     4.295   0.938   8.717  1.00 24.46          C
ATOM   1379  CE2 TRP A 505     4.834   1.808   7.739  1.00 23.54          C
ATOM   1380  CE3 TRP A 505     5.155   0.383   9.681  1.00 26.35          C
ATOM   1381  CD1 TRP A 505     2.633   1.615   7.365  1.00 19.83          C
ATOM   1382  NE1 TRP A 505     3.801   2.208   6.926  1.00 24.61          N
ATOM   1383  CZ2 TRP A 505     6.198   2.138   7.692  1.00 27.89          C
ATOM   1384  CZ3 TRP A 505     6.516   0.709   9.635  1.00 27.25          C
ATOM   1385  CH2 TRP A 505     7.024   1.581   8.642  1.00 26.23          C
ATOM   1386  C   TRP A 505     0.070   0.305  10.971  1.00 22.11          C
ATOM   1387  O   TRP A 505    -0.926   0.429  10.258  1.00 22.39          O
ATOM   1388  N   TYR A 506     0.027  -0.266  12.167  1.00 21.52          N
ATOM   1389  CA  TYR A 506    -1.231  -0.889  12.650  1.00 22.86          C
ATOM   1390  CB  TYR A 506    -0.859  -2.165  13.442  1.00 21.24          C
ATOM   1391  CG  TYR A 506    -0.540  -3.393  12.593  1.00 23.75          C
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ATOM   1392  CD1 TYR A 506     -0.335  -3.297  11.221  1.00 25.21           C
ATOM   1393  CE1 TYR A 506     -0.008  -4.434  10.444  1.00 33.36           C
ATOM   1394  CD2 TYR A 506     -0.424  -4.659  13.184  1.00 30.33           C
ATOM   1395  CE2 TYR A 506     -0.113  -5.795  12.413  1.00 33.98           C
ATOM   1396  CZ  TYR A 506      0.100  -5.674  11.053  1.00 34.14           C
ATOM   1397  OH  TYR A 506      0.459  -6.784  10.310  1.00 36.03           O
ATOM   1398  C   TYR A 506     -2.184  -0.017  13.500  1.00 25.61           C
ATOM   1399  O   TYR A 506     -1.737   0.682  14.412  1.00 24.59           O
ATOM   1400  N   ALA A 507     -3.490  -0.076  13.209  1.00 21.31           N
ATOM   1401  CA  ALA A 507     -4.511   0.664  13.950  1.00 21.80           C
ATOM   1402  CB  ALA A 507     -5.894   0.502  13.254  1.00 18.75           C
ATOM   1403  C   ALA A 507     -4.570   0.070  15.374  1.00 26.17           C
ATOM   1404  O   ALA A 507     -4.161  -1.064  15.607  1.00 22.46           O
ATOM   1405  N   PRO A 508     -5.107   0.831  16.332  1.00 22.10           N
ATOM   1406  CD  PRO A 508     -5.596   2.214  16.186  1.00 22.87           C
ATOM   1407  CA  PRO A 508     -5.213   0.370  17.722  1.00 24.97           C
ATOM   1408  CB  PRO A 508     -5.979   1.499  18.403  1.00 25.74           C
ATOM   1409  CG  PRO A 508     -5.555   2.711  17.600  1.00 34.90           C
ATOM   1410  C   PRO A 508     -5.898  -0.978  17.922  1.00 28.04           C
ATOM   1411  O   PRO A 508     -5.397  -1.819  18.682  1.00 24.23           O
ATOM   1412  N   GLU A 509     -7.019  -1.193  17.229  1.00 24.59           N
ATOM   1413  CA  GLU A 509     -7.754  -2.445  17.352  1.00 27.89           C
ATOM   1414  CB  GLU A 509     -9.128  -2.368  16.654  1.00 27.01           C
ATOM   1415  CG  GLU A 509     -9.060  -2.329  15.121  1.00 23.52           C
ATOM   1416  CD  GLU A 509     -8.971  -0.909  14.578  1.00 30.32           C
ATOM   1417  OE1 GLU A 509     -8.712   0.038  15.366  1.00 23.83           O
ATOM   1418  OE2 GLU A 509     -9.139  -0.750  13.346  1.00 24.89           O
ATOM   1419  C   GLU A 509     -6.954  -3.636  16.829  1.00 24.33           C
ATOM   1420  O   GLU A 509     -7.196  -4.767  17.246  1.00 24.26           O
ATOM   1421  N   CYS A 510     -6.009  -3.391  15.913  1.00 20.72           N
ATOM   1422  CA  CYS A 510     -5.173  -4.456  15.392  1.00 18.85           C
ATOM   1423  CB  CYS A 510     -4.314  -3.963  14.213  1.00 20.67           C
ATOM   1424  SG  CYS A 510     -5.287  -3.330  12.822  1.00 25.10           S
ATOM   1425  C   CYS A 510     -4.216  -4.926  16.503  1.00 21.45           C
ATOM   1426  O   CYS A 510     -4.026  -6.104  16.720  1.00 24.61           O
ATOM   1427  N   ILE A 511     -3.590  -3.972  17.164  1.00 22.33           N
ATOM   1428  CA  ILE A 511     -2.629  -4.304  18.208  1.00 27.31           C
ATOM   1429  CB  ILE A 511     -1.724  -3.081  18.537  1.00 27.85           C
ATOM   1430  CG2 ILE A 511     -0.701  -3.445  19.641  1.00 32.87           C
ATOM   1431  CG1 ILE A 511     -1.004  -2.638  17.255  1.00 27.31           C
ATOM   1432  CD1 ILE A 511     -0.335  -1.270  17.338  1.00 34.56           C
ATOM   1433  C   ILE A 511     -3.318  -4.797  19.475  1.00 31.42           C
ATOM   1434  O   ILE A 511     -2.887  -5.791  20.071  1.00 29.83           O
ATOM   1435  N   ASN A 512     -4.413  -4.152  19.861  1.00 24.92           N
ATOM   1436  CA  ASN A 512     -5.068  -4.547  21.093  1.00 27.73           C
ATOM   1437  CB  ASN A 512     -5.860  -3.387  21.681  1.00 24.36           C
ATOM   1438  CG  ASN A 512     -4.980  -2.240  22.108  1.00 34.57           C
ATOM   1439  OD1 ASN A 512     -3.903  -2.442  22.653  1.00 38.07           O
ATOM   1440  ND2 ASN A 512     -5.447  -1.024  21.872  1.00 38.61           N
ATOM   1441  C   ASN A 512     -5.973  -5.747  20.953  1.00 30.41           C
ATOM   1442  O   ASN A 512     -6.100  -6.530  21.893  1.00 30.25           O
ATOM   1443  N   PHE A 513     -6.622  -5.898  19.804  1.00 23.64           N
ATOM   1444  CA  PHE A 513     -7.529  -7.031  19.648  1.00 23.12           C
ATOM   1445  CB  PHE A 513     -8.965  -6.544  19.642  1.00 24.06           C
ATOM   1446  CG  PHE A 513     -9.365  -5.836  20.901  1.00 33.74           C
ATOM   1447  CD1 PHE A 513     -9.502  -4.456  20.925  1.00 33.94           C
ATOM   1448  CD2 PHE A 513     -9.566  -6.558  22.081  1.00 33.20           C
ATOM   1449  CE1 PHE A 513     -9.829  -3.790  22.119  1.00 40.69           C
ATOM   1450  CE2 PHE A 513     -9.894  -5.901  23.267  1.00 39.14           C
ATOM   1451  CZ  PHE A 513    -10.021  -4.517  23.282  1.00 38.17           C
ATOM   1452  C   PHE A 513     -7.299  -7.940  18.447  1.00 26.12           C
ATOM   1453  O   PHE A 513     -8.122  -8.815  18.183  1.00 25.90           O
ATOM   1454  N   ARG A 514     -6.200  -7.719  17.715  1.00 20.92           N
ATOM   1455  CA  ARG A 514     -5.855  -8.511  16.548  1.00 18.78           C
ATOM   1456  CB  ARG A 514     -5.504  -9.966  16.974  1.00 22.53           C
ATOM   1457  CG  ARG A 514     -4.403  -9.980  18.017  1.00 24.16           C
ATOM   1458  CD  ARG A 514     -3.883 -11.364  18.353  1.00 26.16           C
ATOM   1459  NE  ARG A 514     -2.727 -11.229  19.247  1.00 25.10           N
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ATOM   1460  CZ   ARG A 514    -1.983  -12.248  19.657  1.00 27.44      C
ATOM   1461  NH1  ARG A 514    -2.269  -13.477  19.264  1.00 27.42      N
ATOM   1462  NH2  ARG A 514    -0.928  -12.027  20.443  1.00 29.69      N
ATOM   1463  C    ARG A 514    -7.008   -8.520  15.532  1.00 19.73      C
ATOM   1464  O    ARG A 514    -7.173   -9.487  14.790  1.00 21.31      O
ATOM   1465  N    LYS A 515    -7.733   -7.404  15.480  1.00 22.26      N
ATOM   1466  CA   LYS A 515    -8.891   -7.277  14.597  1.00 19.38      C
ATOM   1467  CB   LYS A 515    -9.995   -6.589  15.385  1.00 23.23      C
ATOM   1468  CG   LYS A 515   -11.303   -6.407  14.627  1.00 24.88      C
ATOM   1469  CD   LYS A 515   -12.277   -5.554  15.432  1.00 31.97      C
ATOM   1470  CE   LYS A 515   -13.434   -5.099  14.557  1.00 37.46      C
ATOM   1471  NZ   LYS A 515   -14.341   -4.148  15.261  1.00 42.53      N
ATOM   1472  C    LYS A 515    -8.547   -6.460  13.322  1.00 21.36      C
ATOM   1473  O    LYS A 515    -8.165   -5.303  13.436  1.00 20.92      O
ATOM   1474  N    PHE A 516    -8.740   -7.059  12.143  1.00 21.89      N
ATOM   1475  CA   PHE A 516    -8.421   -6.387  10.870  1.00 21.28      C
ATOM   1476  CB   PHE A 516    -7.346   -7.180  10.127  1.00 20.51      C
ATOM   1477  CG   PHE A 516    -6.025   -7.215  10.878  1.00 21.58      C
ATOM   1478  CD1  PHE A 516    -5.857   -8.098  11.954  1.00 23.48      C
ATOM   1479  CD2  PHE A 516    -4.998   -6.338  10.555  1.00 23.31      C
ATOM   1480  CE1  PHE A 516    -4.672   -8.099  12.698  1.00 25.88      C
ATOM   1481  CE2  PHE A 516    -3.814   -6.334  11.296  1.00 24.06      C
ATOM   1482  CZ   PHE A 516    -3.654   -7.220  12.370  1.00 29.09      C
ATOM   1483  C    PHE A 516    -9.659   -6.196  10.014  1.00 24.42      C
ATOM   1484  O    PHE A 516   -10.584   -7.031  10.045  1.00 21.09      O
ATOM   1485  N    SER A 517    -9.648   -5.111   9.241  1.00 20.69      N
ATOM   1486  CA   SER A 517   -10.818   -4.718   8.434  1.00 26.64      C
ATOM   1487  CB   SER A 517   -11.826   -4.042   9.379  1.00 21.54      C
ATOM   1488  OG   SER A 517   -11.213   -2.897  10.008  1.00 22.44      O
ATOM   1489  C    SER A 517   -10.377   -3.679   7.393  1.00 21.26      C
ATOM   1490  O    SER A 517    -9.236   -3.288   7.397  1.00 19.96      O
ATOM   1491  N    SER A 518   -11.287   -3.223   6.529  1.00 19.99      N
ATOM   1492  CA   SER A 518   -10.873   -2.180   5.589  1.00 20.05      C
ATOM   1493  CB   SER A 518   -12.002   -1.884   4.584  1.00 27.16      C
ATOM   1494  OG   SER A 518   -12.033   -2.959   3.646  1.00 30.81      O
ATOM   1495  C    SER A 518   -10.473   -0.946   6.366  1.00 19.52      C
ATOM   1496  O    SER A 518    -9.591   -0.196   5.937  1.00 26.21      O
ATOM   1497  N    ARG A 519   -11.119   -0.725   7.500  1.00 22.21      N
ATOM   1498  CA   ARG A 519   -10.780    0.414   8.311  1.00 18.10      C
ATOM   1499  CB   ARG A 519   -11.842    0.646   9.371  1.00 22.77      C
ATOM   1500  CG   ARG A 519   -13.023    1.415   8.764  1.00 25.96      C
ATOM   1501  CD   ARG A 519   -14.180    1.425   9.709  1.00 34.85      C
ATOM   1502  NE   ARG A 519   -15.279    2.180   9.131  1.00 42.62      N
ATOM   1503  CZ   ARG A 519   -16.510    2.192   9.633  1.00 49.29      C
ATOM   1504  NH1  ARG A 519   -16.798    1.484  10.727  1.00 43.62      N
ATOM   1505  NH2  ARG A 519   -17.458    2.899   9.031  1.00 50.64      N
ATOM   1506  C    ARG A 519    -9.393    0.343   8.939  1.00 20.79      C
ATOM   1507  O    ARG A 519    -8.808    1.403   9.221  1.00 20.53      O
ATOM   1508  N    SER A 520    -8.877   -0.867   9.182  1.00 18.48      N
ATOM   1509  CA   SER A 520    -7.508   -0.904   9.705  1.00 19.17      C
ATOM   1510  CB   SER A 520    -7.177   -2.264  10.410  1.00 17.39      C
ATOM   1511  OG   SER A 520    -7.348   -3.401   9.603  1.00 22.96      O
ATOM   1512  C    SER A 520    -6.586   -0.607   8.484  1.00 18.94      C
ATOM   1513  O    SER A 520    -5.506   -0.023   8.631  1.00 21.65      O
ATOM   1514  N    ASP A 521    -7.032   -0.960   7.272  1.00 19.22      N
ATOM   1515  CA   ASP A 521    -6.261   -0.657   6.038  1.00 23.13      C
ATOM   1516  CB   ASP A 521    -6.902   -1.257   4.770  1.00 27.96      C
ATOM   1517  CG   ASP A 521    -6.488   -2.716   4.501  1.00 23.02      C
ATOM   1518  OD1  ASP A 521    -5.536   -3.223   5.145  1.00 22.00      O
ATOM   1519  OD2  ASP A 521    -7.113   -3.347   3.598  1.00 23.07      O
ATOM   1520  C    ASP A 521    -6.253    0.877   5.874  1.00 18.27      C
ATOM   1521  O    ASP A 521    -5.238    1.473   5.445  1.00 20.55      O
ATOM   1522  N    VAL A 522    -7.366    1.525   6.246  1.00 16.95      N
ATOM   1523  CA   VAL A 522    -7.421    3.004   6.168  1.00 16.30      C
ATOM   1524  CB   VAL A 522    -8.833    3.534   6.537  1.00 18.70      C
ATOM   1525  CG1  VAL A 522    -8.820    5.066   6.757  1.00 19.08      C
ATOM   1526  CG2  VAL A 522    -9.801    3.174   5.395  1.00 15.77      C
ATOM   1527  C    VAL A 522    -6.361    3.620   7.093  1.00 20.10      C
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ATOM   1528  O    VAL A 522    -5.670   4.569   6.711  1.00  19.37        O
ATOM   1529  N    TRP A 523    -6.210   3.069   8.294  1.00  19.01        N
ATOM   1530  CA   TRP A 523    -5.186   3.593   9.216  1.00  17.00        C
ATOM   1531  CB   TRP A 523    -5.240   2.819  10.551  1.00  16.75        C
ATOM   1532  CG   TRP A 523    -4.247   3.339  11.594  1.00  17.47        C
ATOM   1533  CD2  TRP A 523    -4.561   4.078  12.781  1.00  18.40        C
ATOM   1534  CE2  TRP A 523    -3.336   4.384  13.411  1.00  19.18        C
ATOM   1535  CE3  TRP A 523    -5.763   4.514  13.379  1.00  16.68        C
ATOM   1536  CD1  TRP A 523    -2.889   3.226  11.559  1.00  22.45        C
ATOM   1537  NE1  TRP A 523    -2.327   3.856  12.650  1.00  17.34        N
ATOM   1538  CZ2  TRP A 523    -3.267   5.112  14.607  1.00  20.28        C
ATOM   1539  CZ3  TRP A 523    -5.692   5.242  14.570  1.00  18.90        C
ATOM   1540  CH2  TRP A 523    -4.457   5.536  15.170  1.00  20.73        C
ATOM   1541  C    TRP A 523    -3.799   3.464   8.573  1.00  16.27        C
ATOM   1542  O    TRP A 523    -2.988   4.402   8.628  1.00  19.33        O
ATOM   1543  N    SER A 524    -3.528   2.315   7.952  1.00  17.09        N
ATOM   1544  CA   SER A 524    -2.231   2.082   7.277  1.00  22.19        C
ATOM   1545  CB   SER A 524    -2.178   0.658   6.722  1.00  21.77        C
ATOM   1546  OG   SER A 524    -2.247  -0.299   7.751  1.00  31.82        O
ATOM   1547  C    SER A 524    -2.008   3.039   6.114  1.00  23.32        C
ATOM   1548  O    SER A 524    -0.888   3.499   5.878  1.00  17.77        O
ATOM   1549  N    TYR A 525    -3.076   3.334   5.381  1.00  22.60        N
ATOM   1550  CA   TYR A 525    -3.042   4.279   4.274  1.00  22.61        C
ATOM   1551  CB   TYR A 525    -4.457   4.413   3.642  1.00  20.36        C
ATOM   1552  CG   TYR A 525    -4.463   5.402   2.506  1.00  18.97        C
ATOM   1553  CD1  TYR A 525    -3.886   5.077   1.285  1.00  21.53        C
ATOM   1554  CE1  TYR A 525    -3.835   6.020   0.230  1.00  20.51        C
ATOM   1555  CD2  TYR A 525    -5.005   6.685   2.673  1.00  20.00        C
ATOM   1556  CE2  TYR A 525    -4.961   7.620   1.642  1.00  21.87        C
ATOM   1557  CZ   TYR A 525    -4.376   7.284   0.428  1.00  24.64        C
ATOM   1558  OH   TYR A 525    -4.358   8.214  -0.589  1.00  24.81        O
ATOM   1559  C    TYR A 525    -2.590   5.634   4.815  1.00  18.79        C
ATOM   1560  O    TYR A 525    -1.760   6.319   4.208  1.00  22.11        O
ATOM   1561  N    GLY A 526    -3.133   6.036   5.963  1.00  16.47        N
ATOM   1562  CA   GLY A 526    -2.737   7.291   6.582  1.00  17.93        C
ATOM   1563  C    GLY A 526    -1.233   7.343   6.852  1.00  20.82        C
ATOM   1564  O    GLY A 526    -0.571   8.366   6.583  1.00  20.21        O
ATOM   1565  N    VAL A 527    -0.691   6.262   7.409  1.00  18.53        N
ATOM   1566  CA   VAL A 527     0.755   6.202   7.680  1.00  15.75        C
ATOM   1567  CB   VAL A 527     1.109   4.902   8.447  1.00  20.06        C
ATOM   1568  CG1  VAL A 527     2.624   4.842   8.768  1.00  18.66        C
ATOM   1569  CG2  VAL A 527     0.292   4.872   9.769  1.00  19.72        C
ATOM   1570  C    VAL A 527     1.490   6.249   6.326  1.00  16.40        C
ATOM   1571  O    VAL A 527     2.527   6.888   6.205  1.00  21.73        O
ATOM   1572  N    THR A 528     0.941   5.594   5.307  1.00  19.11        N
ATOM   1573  CA   THR A 528     1.562   5.595   3.975  1.00  18.53        C
ATOM   1574  CB   THR A 528     0.794   4.663   3.020  1.00  21.20        C
ATOM   1575  OG1  THR A 528     0.891   3.318   3.519  1.00  21.69        O
ATOM   1576  CG2  THR A 528     1.392   4.705   1.618  1.00  22.45        C
ATOM   1577  C    THR A 528     1.587   7.032   3.416  1.00  24.70        C
ATOM   1578  O    THR A 528     2.599   7.456   2.850  1.00  19.73        O
ATOM   1579  N    MET A 529     0.479   7.764   3.587  1.00  19.61        N
ATOM   1580  CA   MET A 529     0.425   9.179   3.143  1.00  19.25        C
ATOM   1581  CB   MET A 529    -0.902   9.848   3.576  1.00  20.84        C
ATOM   1582  CG   MET A 529    -2.135   9.296   2.846  1.00  22.24        C
ATOM   1583  SD   MET A 529    -3.608  10.284   3.352  1.00  24.00        S
ATOM   1584  CE   MET A 529    -3.207  11.921   2.622  1.00  23.54        C
ATOM   1585  C    MET A 529     1.560   9.943   3.821  1.00  19.48        C
ATOM   1586  O    MET A 529     2.276  10.736   3.182  1.00  20.92        O
ATOM   1587  N    TRP A 530     1.724   9.726   5.124  1.00  19.75        N
ATOM   1588  CA   TRP A 530     2.777  10.434   5.882  1.00  18.54        C
ATOM   1589  CB   TRP A 530     2.731  10.069   7.376  1.00  20.48        C
ATOM   1590  CG   TRP A 530     3.582  10.944   8.225  1.00  18.20        C
ATOM   1591  CD2  TRP A 530     4.969  10.745   8.527  1.00  18.21        C
ATOM   1592  CE2  TRP A 530     5.389  11.838   9.336  1.00  19.74        C
ATOM   1593  CE3  TRP A 530     5.899   9.752   8.197  1.00  20.68        C
ATOM   1594  CD1  TRP A 530     3.214  12.116   8.842  1.00  18.28        C
ATOM   1595  NE1  TRP A 530     4.305  12.661   9.520  1.00  22.22        N
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ATOM	1596	CZ2	TRP	A	530	6.712	11.961	9.819	1.00	25.36	C
ATOM	1597	CZ3	TRP	A	530	7.212	9.872	8.681	1.00	22.68	C
ATOM	1598	CH2	TRP	A	530	7.598	10.969	9.479	1.00	26.97	C
ATOM	1599	C	TRP	A	530	4.171	10.152	5.349	1.00	21.37	C
ATOM	1600	O	TRP	A	530	4.972	11.093	5.118	1.00	22.21	O
ATOM	1601	N	GLU	A	531	4.475	8.870	5.161	1.00	22.41	N
ATOM	1602	CA	GLU	A	531	5.773	8.443	4.634	1.00	23.01	C
ATOM	1603	CB	GLU	A	531	5.800	6.938	4.345	1.00	22.19	C
ATOM	1604	CG	GLU	A	531	5.636	5.990	5.540	1.00	26.83	C
ATOM	1605	CD	GLU	A	531	5.699	4.530	5.079	1.00	29.43	C
ATOM	1606	OE1	GLU	A	531	4.621	3.926	4.848	1.00	23.48	O
ATOM	1607	OE2	GLU	A	531	6.836	3.999	4.921	1.00	26.99	O
ATOM	1608	C	GLU	A	531	6.035	9.114	3.304	1.00	22.15	C
ATOM	1609	O	GLU	A	531	7.149	9.587	3.030	1.00	22.47	O
ATOM	1610	N	ALA	A	532	5.017	9.120	2.445	1.00	20.60	N
ATOM	1611	CA	ALA	A	532	5.170	9.710	1.121	1.00	20.49	C
ATOM	1612	CB	ALA	A	532	3.951	9.366	0.222	1.00	21.29	C
ATOM	1613	C	ALA	A	532	5.376	11.209	1.143	1.00	22.68	C
ATOM	1614	O	ALA	A	532	6.294	11.721	0.487	1.00	21.66	O
ATOM	1615	N	LEU	A	533	4.523	11.918	1.881	1.00	24.52	N
ATOM	1616	CA	LEU	A	533	4.601	13.377	1.957	1.00	27.55	C
ATOM	1617	CB	LEU	A	533	3.301	13.951	2.553	1.00	23.33	C
ATOM	1618	CG	LEU	A	533	2.113	13.809	1.586	1.00	24.16	C
ATOM	1619	CD1	LEU	A	533	0.784	14.069	2.314	1.00	30.47	C
ATOM	1620	CD2	LEU	A	533	2.289	14.808	0.408	1.00	26.48	C
ATOM	1621	C	LEU	A	533	5.832	13.849	2.737	1.00	28.49	C
ATOM	1622	O	LEU	A	533	6.213	15.021	2.661	1.00	23.09	O
ATOM	1623	N	SER	A	534	6.458	12.921	3.462	1.00	23.64	N
ATOM	1624	CA	SER	A	534	7.686	13.216	4.218	1.00	24.10	C
ATOM	1625	CB	SER	A	534	7.717	12.409	5.509	1.00	24.84	C
ATOM	1626	OG	SER	A	534	6.724	12.875	6.402	1.00	32.38	O
ATOM	1627	C	SER	A	534	8.867	12.778	3.370	1.00	23.66	C
ATOM	1628	O	SER	A	534	10.004	12.749	3.839	1.00	26.17	O
ATOM	1629	N	TYR	A	535	8.581	12.408	2.130	1.00	23.34	N
ATOM	1630	CA	TYR	A	535	9.593	11.943	1.196	1.00	28.19	C
ATOM	1631	CB	TYR	A	535	10.485	13.112	0.733	1.00	28.89	C
ATOM	1632	CG	TYR	A	535	9.724	14.020	-0.219	1.00	29.59	C
ATOM	1633	CD1	TYR	A	535	8.811	14.939	0.274	1.00	28.98	C
ATOM	1634	CE1	TYR	A	535	8.026	15.712	-0.584	1.00	30.80	C
ATOM	1635	CD2	TYR	A	535	9.849	13.887	-1.599	1.00	26.41	C
ATOM	1636	CE2	TYR	A	535	9.063	14.647	-2.472	1.00	29.12	C
ATOM	1637	CZ	TYR	A	535	8.155	15.558	-1.948	1.00	23.83	C
ATOM	1638	OH	TYR	A	535	7.383	16.325	-2.773	1.00	30.19	O
ATOM	1639	C	TYR	A	535	10.447	10.781	1.709	1.00	32.28	C
ATOM	1640	O	TYR	A	535	11.672	10.845	1.691	1.00	27.48	O
ATOM	1641	N	GLY	A	536	9.781	9.722	2.174	1.00	26.27	N
ATOM	1642	CA	GLY	A	536	10.495	8.530	2.610	1.00	25.77	C
ATOM	1643	C	GLY	A	536	11.019	8.433	4.022	1.00	30.26	C
ATOM	1644	O	GLY	A	536	11.754	7.499	4.353	1.00	37.11	O
ATOM	1645	N	GLN	A	537	10.648	9.380	4.876	1.00	30.46	N
ATOM	1646	CA	GLN	A	537	11.080	9.346	6.263	1.00	28.08	C
ATOM	1647	CB	GLN	A	537	10.740	10.672	6.935	1.00	34.05	C
ATOM	1648	CG	GLN	A	537	11.750	11.776	6.618	1.00	44.08	C
ATOM	1649	CD	GLN	A	537	11.367	13.123	7.203	1.00	46.85	C
ATOM	1650	OE1	GLN	A	537	10.983	13.224	8.371	1.00	55.73	O
ATOM	1651	NE2	GLN	A	537	11.477	14.170	6.394	1.00	50.81	N
ATOM	1652	C	GLN	A	537	10.401	8.188	7.011	1.00	29.96	C
ATOM	1653	O	GLN	A	537	9.343	7.715	6.601	1.00	24.20	O
ATOM	1654	N	LYS	A	538	11.028	7.722	8.094	1.00	26.82	N
ATOM	1655	CA	LYS	A	538	10.446	6.638	8.870	1.00	27.30	C
ATOM	1656	CB	LYS	A	538	11.533	5.871	9.635	1.00	32.27	C
ATOM	1657	CG	LYS	A	538	12.495	5.132	8.724	1.00	41.48	C
ATOM	1658	CD	LYS	A	538	13.536	4.359	9.529	1.00	46.01	C
ATOM	1659	CE	LYS	A	538	14.278	3.365	8.644	1.00	48.76	C
ATOM	1660	NZ	LYS	A	538	15.278	2.577	9.429	1.00	54.95	N
ATOM	1661	C	LYS	A	538	9.431	7.175	9.875	1.00	28.24	C
ATOM	1662	O	LYS	A	538	9.665	8.195	10.529	1.00	28.85	O
ATOM	1663	N	PRO	A	539	8.283	6.496	10.008	1.00	24.53	N

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ATOM	1664	CD	PRO	A	539	7.742	5.389	9.198	1.00	22.29	C
ATOM	1665	CA	PRO	A	539	7.286	6.966	10.972	1.00	24.04	C
ATOM	1666	CB	PRO	A	539	6.053	6.118	10.644	1.00	28.10	C
ATOM	1667	CG	PRO	A	539	6.644	4.857	10.098	1.00	36.04	C
ATOM	1668	C	PRO	A	539	7.737	6.759	12.421	1.00	28.35	C
ATOM	1669	O	PRO	A	539	8.426	5.783	12.734	1.00	25.90	O
ATOM	1670	N	TYR	A	540	7.343	7.680	13.292	1.00	23.53	N
ATOM	1671	CA	TYR	A	540	7.656	7.645	14.722	1.00	28.38	C
ATOM	1672	CB	TYR	A	540	6.831	6.555	15.418	1.00	24.00	C
ATOM	1673	CG	TYR	A	540	5.331	6.586	15.095	1.00	27.38	C
ATOM	1674	CD1	TYR	A	540	4.477	7.452	15.766	1.00	24.16	C
ATOM	1675	CE1	TYR	A	540	3.096	7.476	15.483	1.00	20.41	C
ATOM	1676	CD2	TYR	A	540	4.800	5.746	14.119	1.00	28.23	C
ATOM	1677	CE2	TYR	A	540	3.417	5.767	13.800	1.00	21.95	C
ATOM	1678	CZ	TYR	A	540	2.580	6.632	14.496	1.00	20.01	C
ATOM	1679	OH	TYR	A	540	1.244	6.670	14.207	1.00	24.93	O
ATOM	1680	C	TYR	A	540	9.136	7.346	14.903	1.00	28.93	C
ATOM	1681	O	TYR	A	540	9.508	6.478	15.689	1.00	30.14	O
ATOM	1682	N	LYS	A	541	9.942	8.095	14.152	1.00	27.25	N
ATOM	1683	CA	LYS	A	541	11.391	7.985	14.100	1.00	39.82	C
ATOM	1684	CB	LYS	A	541	11.939	9.274	13.472	1.00	44.06	C
ATOM	1685	CG	LYS	A	541	13.334	9.167	12.893	1.00	54.68	C
ATOM	1686	CD	LYS	A	541	13.699	10.418	12.075	1.00	54.79	C
ATOM	1687	CE	LYS	A	541	12.794	10.586	10.848	1.00	59.69	C
ATOM	1688	NZ	LYS	A	541	13.234	11.695	9.938	1.00	56.19	N
ATOM	1689	C	LYS	A	541	12.074	7.722	15.447	1.00	42.70	C
ATOM	1690	O	LYS	A	541	12.849	6.777	15.590	1.00	43.82	O
ATOM	1691	N	LYS	A	542	11.784	8.549	16.433	1.00	44.10	N
ATOM	1692	CA	LYS	A	542	12.425	8.378	17.728	1.00	51.64	C
ATOM	1693	CB	LYS	A	542	12.682	9.749	18.350	1.00	51.94	C
ATOM	1694	CG	LYS	A	542	11.425	10.565	18.581	1.00	56.75	C
ATOM	1695	CD	LYS	A	542	11.731	11.841	19.359	1.00	59.67	C
ATOM	1696	CE	LYS	A	542	10.445	12.559	19.767	1.00	60.04	C
ATOM	1697	NZ	LYS	A	542	10.684	13.819	20.538	1.00	63.82	N
ATOM	1698	C	LYS	A	542	11.649	7.512	18.709	1.00	55.84	C
ATOM	1699	O	LYS	A	542	11.746	7.724	19.920	1.00	59.11	O
ATOM	1700	N	MET	A	543	10.908	6.523	18.207	1.00	41.98	N
ATOM	1701	CA	MET	A	543	10.125	5.658	19.083	1.00	43.90	C
ATOM	1702	CB	MET	A	543	8.645	6.029	19.019	1.00	45.70	C
ATOM	1703	CG	MET	A	543	8.230	7.209	19.856	1.00	53.80	C
ATOM	1704	SD	MET	A	543	6.477	7.548	19.578	1.00	44.32	S
ATOM	1705	CE	MET	A	543	6.609	9.128	18.721	1.00	44.97	C
ATOM	1706	C	MET	A	543	10.235	4.185	18.755	1.00	46.16	C
ATOM	1707	O	MET	A	543	10.497	3.805	17.616	1.00	49.81	O
ATOM	1708	N	LYS	A	544	10.001	3.359	19.769	1.00	48.84	N
ATOM	1709	CA	LYS	A	544	10.042	1.909	19.627	1.00	54.57	C
ATOM	1710	CB	LYS	A	544	10.872	1.284	20.748	1.00	54.75	C
ATOM	1711	CG	LYS	A	544	10.262	1.451	22.134	1.00	63.19	C
ATOM	1712	CD	LYS	A	544	11.076	0.704	23.191	1.00	63.73	C
ATOM	1713	CE	LYS	A	544	10.400	0.726	24.560	1.00	65.53	C
ATOM	1714	NZ	LYS	A	544	11.146	-0.103	25.561	1.00	62.21	N
ATOM	1715	C	LYS	A	544	8.612	1.374	19.699	1.00	57.82	C
ATOM	1716	O	LYS	A	544	7.655	2.112	19.464	1.00	56.73	O
ATOM	1717	N	GLY	A	545	8.475	0.096	20.046	1.00	53.41	N
ATOM	1718	CA	GLY	A	545	7.161	-0.512	20.128	1.00	51.20	C
ATOM	1719	C	GLY	A	545	6.218	0.124	21.133	1.00	51.82	C
ATOM	1720	O	GLY	A	545	5.359	0.915	20.752	1.00	53.88	O
ATOM	1721	N	PRO	A	546	6.350	-0.206	22.427	1.00	52.05	N
ATOM	1722	CD	PRO	A	546	7.333	-1.165	22.966	1.00	55.28	C
ATOM	1723	CA	PRO	A	546	5.507	0.321	23.506	1.00	51.30	C
ATOM	1724	CB	PRO	A	546	6.215	-0.181	24.768	1.00	52.03	C
ATOM	1725	CG	PRO	A	546	6.743	-1.503	24.322	1.00	51.79	C
ATOM	1726	C	PRO	A	546	5.325	1.835	23.515	1.00	44.10	C
ATOM	1727	O	PRO	A	546	4.296	2.342	23.983	1.00	37.86	O
ATOM	1728	N	GLU	A	547	6.329	2.553	23.017	1.00	39.18	N
ATOM	1729	CA	GLU	A	547	6.274	4.004	22.973	1.00	45.81	C
ATOM	1730	CB	GLU	A	547	7.607	4.582	22.516	1.00	44.80	C
ATOM	1731	CG	GLU	A	547	8.760	4.296	23.450	1.00	60.26	C

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ATOM   1732  CD  GLU A 547     10.033   4.970  23.001  1.00 56.95           C
ATOM   1733  OE1 GLU A 547     10.093   6.220  23.034  1.00 61.75           O
ATOM   1734  OE2 GLU A 547     10.970   4.247  22.608  1.00 59.24           O
ATOM   1735  C   GLU A 547      5.173   4.495  22.030  1.00 31.92           C
ATOM   1736  O   GLU A 547      4.417   5.381  22.384  1.00 33.88           O
ATOM   1737  N   VAL A 548      5.113   3.922  20.834  1.00 36.76           N
ATOM   1738  CA  VAL A 548      4.097   4.331  19.849  1.00 30.35           C
ATOM   1739  CB  VAL A 548      4.316   3.610  18.513  1.00 35.20           C
ATOM   1740  CG1 VAL A 548      3.289   4.083  17.486  1.00 31.70           C
ATOM   1741  CG2 VAL A 548      5.723   3.888  18.016  1.00 39.20           C
ATOM   1742  C   VAL A 548      2.678   4.060  20.344  1.00 32.59           C
ATOM   1743  O   VAL A 548      1.801   4.913  20.242  1.00 32.29           O
ATOM   1744  N   MET A 549      2.448   2.874  20.899  1.00 34.32           N
ATOM   1745  CA  MET A 549      1.131   2.528  21.418  1.00 33.89           C
ATOM   1746  CB  MET A 549      1.171   1.125  22.025  1.00 43.40           C
ATOM   1747  CG  MET A 549     -0.202   0.486  22.120  1.00 54.00           C
ATOM   1748  SD  MET A 549     -1.061   0.474  20.506  1.00 73.10           S
ATOM   1749  CE  MET A 549     -2.239   1.839  20.656  1.00 53.85           C
ATOM   1750  C   MET A 549      0.650   3.532  22.476  1.00 31.82           C
ATOM   1751  O   MET A 549     -0.486   4.000  22.436  1.00 30.85           O
ATOM   1752  N   ALA A 550      1.525   3.856  23.420  1.00 30.61           N
ATOM   1753  CA  ALA A 550      1.194   4.791  24.490  1.00 32.54           C
ATOM   1754  CB  ALA A 550      2.363   4.852  25.488  1.00 37.38           C
ATOM   1755  C   ALA A 550      0.910   6.186  23.911  1.00 27.78           C
ATOM   1756  O   ALA A 550      0.004   6.894  24.362  1.00 28.75           O
ATOM   1757  N   PHE A 551      1.711   6.569  22.920  1.00 26.75           N
ATOM   1758  CA  PHE A 551      1.595   7.861  22.220  1.00 29.08           C
ATOM   1759  CB  PHE A 551      2.712   7.922  21.157  1.00 21.20           C
ATOM   1760  CG  PHE A 551      2.791   9.219  20.382  1.00 25.99           C
ATOM   1761  CD1 PHE A 551      3.346  10.358  20.954  1.00 30.16           C
ATOM   1762  CD2 PHE A 551      2.370   9.265  19.041  1.00 29.19           C
ATOM   1763  CE1 PHE A 551      3.497  11.540  20.206  1.00 26.26           C
ATOM   1764  CE2 PHE A 551      2.521  10.449  18.286  1.00 24.90           C
ATOM   1765  CZ  PHE A 551      3.087  11.577  18.877  1.00 28.07           C
ATOM   1766  C   PHE A 551      0.214   7.955  21.565  1.00 23.03           C
ATOM   1767  O   PHE A 551     -0.516   8.922  21.748  1.00 24.86           O
ATOM   1768  N   ILE A 552     -0.149   6.931  20.806  1.00 23.91           N
ATOM   1769  CA  ILE A 552     -1.452   6.917  20.145  1.00 23.84           C
ATOM   1770  CB  ILE A 552     -1.559   5.675  19.241  1.00 24.60           C
ATOM   1771  CG2 ILE A 552     -2.973   5.513  18.716  1.00 26.02           C
ATOM   1772  CG1 ILE A 552     -0.476   5.757  18.155  1.00 28.63           C
ATOM   1773  CD1 ILE A 552     -0.614   6.952  17.164  1.00 28.18           C
ATOM   1774  C   ILE A 552     -2.575   6.921  21.184  1.00 24.71           C
ATOM   1775  O   ILE A 552     -3.565   7.653  21.048  1.00 25.03           O
ATOM   1776  N   GLU A 553     -2.419   6.121  22.238  1.00 26.97           N
ATOM   1777  CA  GLU A 553     -3.433   6.055  23.295  1.00 27.80           C
ATOM   1778  CB  GLU A 553     -3.040   5.014  24.346  1.00 39.68           C
ATOM   1779  CG  GLU A 553     -3.089   3.573  23.834  1.00 47.86           C
ATOM   1780  CD  GLU A 553     -4.506   3.085  23.586  1.00 47.67           C
ATOM   1781  OE1 GLU A 553     -4.662   2.019  22.950  1.00 54.95           O
ATOM   1782  OE2 GLU A 553     -5.460   3.758  24.032  1.00 55.56           O
ATOM   1783  C   GLU A 553     -3.645   7.424  23.972  1.00 27.09           C
ATOM   1784  O   GLU A 553     -4.757   7.751  24.386  1.00 33.91           O
ATOM   1785  N   GLN A 554     -2.577   8.206  24.088  1.00 30.97           N
ATOM   1786  CA  GLN A 554     -2.639   9.545  24.678  1.00 31.06           C
ATOM   1787  CB  GLN A 554     -1.232  10.093  24.909  1.00 33.93           C
ATOM   1788  CG  GLN A 554     -0.454   9.441  26.030  1.00 47.13           C
ATOM   1789  CD  GLN A 554      0.949   9.978  26.069  1.00 48.57           C
ATOM   1790  OE1 GLN A 554      1.159  11.187  25.932  1.00 53.53           O
ATOM   1791  NE2 GLN A 554      1.921   9.089  26.250  1.00 53.00           N
ATOM   1792  C   GLN A 554     -3.364  10.534  23.767  1.00 34.15           C
ATOM   1793  O   GLN A 554     -3.599  11.677  24.155  1.00 29.68           O
ATOM   1794  N   GLY A 555     -3.698  10.104  22.552  1.00 28.32           N
ATOM   1795  CA  GLY A 555     -4.389  11.008  21.644  1.00 30.45           C
ATOM   1796  C   GLY A 555     -3.449  11.876  20.805  1.00 27.04           C
ATOM   1797  O   GLY A 555     -3.859  12.914  20.269  1.00 28.32           O
ATOM   1798  N   LYS A 556     -2.188  11.478  20.694  1.00 21.48           N
ATOM   1799  CA  LYS A 556     -1.240  12.239  19.886  1.00 21.96           C
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ATOM  1800  CB  LYS A 556    0.096  12.390  20.618  1.00 22.25      C
ATOM  1801  CG  LYS A 556   -0.048  13.123  21.964  1.00 24.42      C
ATOM  1802  CD  LYS A 556    1.312  13.380  22.586  1.00 25.86      C
ATOM  1803  CE  LYS A 556    1.157  14.112  23.934  1.00 34.77      C
ATOM  1804  NZ  LYS A 556    2.485  14.453  24.554  1.00 33.67      N
ATOM  1805  C   LYS A 556   -1.007  11.516  18.567  1.00 23.68      C
ATOM  1806  O   LYS A 556   -1.140  10.291  18.492  1.00 22.12      O
ATOM  1807  N   ARG A 557   -0.610  12.285  17.548  1.00 19.92      N
ATOM  1808  CA  ARG A 557   -0.365  11.722  16.229  1.00 20.32      C
ATOM  1809  CB  ARG A 557   -1.575  11.983  15.311  1.00 20.48      C
ATOM  1810  CG  ARG A 557   -2.895  11.354  15.818  1.00 21.21      C
ATOM  1811  CD  ARG A 557   -2.900   9.812  15.730  1.00 19.93      C
ATOM  1812  NE  ARG A 557   -4.203   9.222  16.106  1.00 19.69      N
ATOM  1813  CZ  ARG A 557   -4.580   8.900  17.343  1.00 22.33      C
ATOM  1814  NH1 ARG A 557   -3.755   9.098  18.397  1.00 21.75      N
ATOM  1815  NH2 ARG A 557   -5.771   8.337  17.536  1.00 19.39      N
ATOM  1816  C   ARG A 557    0.890  12.335  15.616  1.00 20.01      C
ATOM  1817  O   ARG A 557    1.419  13.342  16.131  1.00 21.06      O
ATOM  1818  N   MET A 558    1.371  11.729  14.526  1.00 23.13      N
ATOM  1819  CA  MET A 558    2.562  12.260  13.862  1.00 24.90      C
ATOM  1820  CB  MET A 558    2.999  11.351  12.710  1.00 20.87      C
ATOM  1821  CG  MET A 558    3.673  10.070  13.153  1.00 26.00      C
ATOM  1822  SD  MET A 558    4.400   9.177  11.757  1.00 25.21      S
ATOM  1823  CE  MET A 558    2.987   8.458  10.949  1.00 19.49      C
ATOM  1824  C   MET A 558    2.287  13.669  13.330  1.00 27.66      C
ATOM  1825  O   MET A 558    1.164  13.992  12.898  1.00 21.51      O
ATOM  1826  N   GLU A 559    3.321  14.503  13.371  1.00 24.36      N
ATOM  1827  CA  GLU A 559    3.230  15.871  12.908  1.00 26.80      C
ATOM  1828  CB  GLU A 559    4.539  16.613  13.219  1.00 33.66      C
ATOM  1829  CG  GLU A 559    5.822  15.788  12.977  1.00 43.05      C
ATOM  1830  CD  GLU A 559    6.068  14.712  14.060  1.00 54.97      C
ATOM  1831  OE1 GLU A 559    6.463  15.072  15.198  1.00 59.07      O
ATOM  1832  OE2 GLU A 559    5.867  13.506  13.774  1.00 44.76      O
ATOM  1833  C   GLU A 559    2.939  15.992  11.417  1.00 27.49      C
ATOM  1834  O   GLU A 559    3.209  15.088  10.642  1.00 27.65      O
ATOM  1835  N   CYS A 560    2.387  17.130  11.026  1.00 22.31      N
ATOM  1836  CA  CYS A 560    2.122  17.377   9.616  1.00 23.70      C
ATOM  1837  CB  CYS A 560    1.293  18.655   9.468  1.00 27.79      C
ATOM  1838  SG  CYS A 560    0.980  19.104   7.751  1.00 30.84      S
ATOM  1839  C   CYS A 560    3.490  17.535   8.905  1.00 29.44      C
ATOM  1840  O   CYS A 560    4.350  18.300   9.351  1.00 29.36      O
ATOM  1841  N   PRO A 561    3.733  16.769   7.825  1.00 29.57      N
ATOM  1842  CD  PRO A 561    2.944  15.629   7.312  1.00 26.67      C
ATOM  1843  CA  PRO A 561    5.018  16.890   7.116  1.00 31.79      C
ATOM  1844  CB  PRO A 561    4.865  15.932   5.933  1.00 29.22      C
ATOM  1845  CG  PRO A 561    3.976  14.837   6.496  1.00 25.42      C
ATOM  1846  C   PRO A 561    5.244  18.319   6.619  1.00 29.76      C
ATOM  1847  O   PRO A 561    4.302  19.055   6.362  1.00 26.53      O
ATOM  1848  N   PRO A 562    6.502  18.728   6.473  1.00 36.98      N
ATOM  1849  CD  PRO A 562    7.740  18.045   6.884  1.00 38.45      C
ATOM  1850  CA  PRO A 562    6.775  20.085   5.994  1.00 38.46      C
ATOM  1851  CB  PRO A 562    8.302  20.140   5.984  1.00 42.62      C
ATOM  1852  CG  PRO A 562    8.674  19.202   7.102  1.00 47.24      C
ATOM  1853  C   PRO A 562    6.177  20.293   4.596  1.00 36.90      C
ATOM  1854  O   PRO A 562    6.268  19.415   3.745  1.00 37.38      O
ATOM  1855  N   GLU A 563    5.550  21.445   4.363  1.00 38.19      N
ATOM  1856  CA  GLU A 563    4.968  21.740   3.048  1.00 43.57      C
ATOM  1857  CB  GLU A 563    6.025  21.554   1.944  1.00 50.62      C
ATOM  1858  CG  GLU A 563    7.282  22.401   2.118  1.00 53.80      C
ATOM  1859  CD  GLU A 563    8.502  21.788   1.429  1.00 62.44      C
ATOM  1860  OE1 GLU A 563    8.457  21.580   0.193  1.00 63.21      O
ATOM  1861  OE2 GLU A 563    9.504  21.509   2.131  1.00 64.48      O
ATOM  1862  C   GLU A 563    3.720  20.924   2.698  1.00 44.24      C
ATOM  1863  O   GLU A 563    3.164  21.068   1.607  1.00 48.48      O
ATOM  1864  N   CYS A 564    3.275  20.048   3.598  1.00 41.39      N
ATOM  1865  CA  CYS A 564    2.060  19.285   3.344  1.00 37.90      C
ATOM  1866  CB  CYS A 564    1.968  18.064   4.279  1.00 37.32      C
ATOM  1867  SG  CYS A 564    0.438  17.119   4.110  1.00 38.37      S
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ATOM	1868	C	CYS	A	564	0.884	20.221	3.602	1.00	37.50	C
ATOM	1869	O	CYS	A	564	0.753	20.773	4.698	1.00	38.57	O
ATOM	1870	N	PRO	A	565	0.012	20.416	2.597	1.00	37.07	N
ATOM	1871	CD	PRO	A	565	0.058	19.780	1.271	1.00	42.57	C
ATOM	1872	CA	PRO	A	565	-1.160	21.294	2.716	1.00	33.51	C
ATOM	1873	CB	PRO	A	565	-1.791	21.231	1.330	1.00	40.30	C
ATOM	1874	CG	PRO	A	565	-1.369	19.883	0.824	1.00	44.48	C
ATOM	1875	C	PRO	A	565	-2.114	20.827	3.792	1.00	35.24	C
ATOM	1876	O	PRO	A	565	-2.258	19.622	4.024	1.00	32.71	O
ATOM	1877	N	PRO	A	566	-2.800	21.776	4.448	1.00	34.52	N
ATOM	1878	CD	PRO	A	566	-2.692	23.231	4.207	1.00	34.66	C
ATOM	1879	CA	PRO	A	566	-3.762	21.487	5.516	1.00	30.97	C
ATOM	1880	CB	PRO	A	566	-4.398	22.862	5.795	1.00	34.13	C
ATOM	1881	CG	PRO	A	566	-3.308	23.823	5.454	1.00	32.16	C
ATOM	1882	C	PRO	A	566	-4.814	20.438	5.135	1.00	34.26	C
ATOM	1883	O	PRO	A	566	-5.149	19.585	5.950	1.00	28.40	O
ATOM	1884	N	GLU	A	567	-5.331	20.498	3.902	1.00	27.60	N
ATOM	1885	CA	GLU	A	567	-6.367	19.562	3.456	1.00	32.42	C
ATOM	1886	CB	GLU	A	567	-6.859	19.918	2.036	1.00	36.27	C
ATOM	1887	CG	GLU	A	567	-6.961	21.413	1.739	1.00	49.38	C
ATOM	1888	CD	GLU	A	567	-5.604	22.059	1.539	1.00	48.16	C
ATOM	1889	OE1	GLU	A	567	-4.880	21.658	0.602	1.00	63.97	O
ATOM	1890	OE2	GLU	A	567	-5.259	22.966	2.318	1.00	48.66	O
ATOM	1891	C	GLU	A	567	-5.848	18.127	3.440	1.00	27.96	C
ATOM	1892	O	GLU	A	567	-6.553	17.189	3.829	1.00	27.68	O
ATOM	1893	N	LEU	A	568	-4.615	17.963	2.976	1.00	24.93	N
ATOM	1894	CA	LEU	A	568	-4.002	16.658	2.906	1.00	28.04	C
ATOM	1895	CB	LEU	A	568	-2.727	16.761	2.076	1.00	31.66	C
ATOM	1896	CG	LEU	A	568	-2.401	15.622	1.133	1.00	34.34	C
ATOM	1897	CD1	LEU	A	568	-3.680	15.015	0.564	1.00	38.44	C
ATOM	1898	CD2	LEU	A	568	-1.519	16.182	0.013	1.00	25.83	C
ATOM	1899	C	LEU	A	568	-3.700	16.146	4.307	1.00	30.03	C
ATOM	1900	O	LEU	A	568	-3.906	14.963	4.591	1.00	26.77	O
ATOM	1901	N	TYR	A	569	-3.199	17.016	5.187	1.00	24.67	N
ATOM	1902	CA	TYR	A	569	-2.947	16.534	6.538	1.00	22.81	C
ATOM	1903	CB	TYR	A	569	-2.176	17.572	7.375	1.00	21.70	C
ATOM	1904	CG	TYR	A	569	-1.824	17.040	8.753	1.00	21.77	C
ATOM	1905	CD1	TYR	A	569	-0.996	15.920	8.895	1.00	23.70	C
ATOM	1906	CE1	TYR	A	569	-0.720	15.375	10.158	1.00	23.93	C
ATOM	1907	CD2	TYR	A	569	-2.371	17.614	9.912	1.00	26.51	C
ATOM	1908	CE2	TYR	A	569	-2.107	17.074	11.184	1.00	29.40	C
ATOM	1909	CZ	TYR	A	569	-1.288	15.960	11.297	1.00	28.24	C
ATOM	1910	OH	TYR	A	569	-1.060	15.430	12.544	1.00	25.64	O
ATOM	1911	C	TYR	A	569	-4.270	16.175	7.234	1.00	23.78	C
ATOM	1912	O	TYR	A	569	-4.326	15.199	7.999	1.00	22.51	O
ATOM	1913	N	ALA	A	570	-5.339	16.936	6.983	1.00	23.61	N
ATOM	1914	CA	ALA	A	570	-6.621	16.634	7.632	1.00	26.10	C
ATOM	1915	CB	ALA	A	570	-7.710	17.646	7.202	1.00	26.46	C
ATOM	1916	C	ALA	A	570	-7.091	15.225	7.308	1.00	24.49	C
ATOM	1917	O	ALA	A	570	-7.666	14.532	8.162	1.00	24.77	O
ATOM	1918	N	LEU	A	571	-6.855	14.806	6.074	1.00	23.99	N
ATOM	1919	CA	LEU	A	571	-7.263	13.499	5.589	1.00	21.89	C
ATOM	1920	CB	LEU	A	571	-7.092	13.432	4.065	1.00	25.02	C
ATOM	1921	CG	LEU	A	571	-7.346	12.049	3.472	1.00	23.70	C
ATOM	1922	CD1	LEU	A	571	-8.724	11.529	3.891	1.00	26.43	C
ATOM	1923	CD2	LEU	A	571	-7.236	12.135	1.953	1.00	26.11	C
ATOM	1924	C	LEU	A	571	-6.406	12.422	6.245	1.00	20.20	C
ATOM	1925	O	LEU	A	571	-6.895	11.428	6.757	1.00	21.42	O
ATOM	1926	N	MET	A	572	-5.105	12.652	6.205	1.00	21.26	N
ATOM	1927	CA	MET	A	572	-4.141	11.758	6.808	1.00	24.72	C
ATOM	1928	CB	MET	A	572	-2.771	12.434	6.700	1.00	30.40	C
ATOM	1929	CG	MET	A	572	-1.685	11.742	7.418	1.00	32.31	C
ATOM	1930	SD	MET	A	572	-0.160	12.660	7.265	1.00	26.55	S
ATOM	1931	CE	MET	A	572	-0.165	13.232	5.451	1.00	24.24	C
ATOM	1932	C	MET	A	572	-4.531	11.574	8.280	1.00	22.05	C
ATOM	1933	O	MET	A	572	-4.607	10.448	8.782	1.00	23.12	O
ATOM	1934	N	SER	A	573	-4.796	12.686	8.965	1.00	18.21	N
ATOM	1935	CA	SER	A	573	-5.158	12.630	10.390	1.00	21.72	C

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ATOM	1936	CB	SER	A	573	-5.155	14.055	10.973	1.00	21.94	C
ATOM	1937	OG	SER	A	573	-5.574	14.093	12.330	1.00	26.24	O
ATOM	1938	C	SER	A	573	-6.498	11.920	10.625	1.00	26.16	C
ATOM	1939	O	SER	A	573	-6.660	11.195	11.599	1.00	21.94	O
ATOM	1940	N	ASP	A	574	-7.471	12.122	9.749	1.00	21.50	N
ATOM	1941	CA	ASP	A	574	-8.748	11.427	9.902	1.00	22.60	C
ATOM	1942	CB	ASP	A	574	-9.791	11.915	8.883	1.00	20.64	C
ATOM	1943	CG	ASP	A	574	-10.332	13.301	9.213	1.00	23.27	C
ATOM	1944	OD1	ASP	A	574	-10.160	13.772	10.360	1.00	22.69	O
ATOM	1945	OD2	ASP	A	574	-10.966	13.888	8.314	1.00	26.93	O
ATOM	1946	C	ASP	A	574	-8.577	9.902	9.750	1.00	22.37	C
ATOM	1947	O	ASP	A	574	-9.359	9.141	10.333	1.00	23.59	O
ATOM	1948	N	CYS	A	575	-7.583	9.453	8.976	1.00	18.61	N
ATOM	1949	CA	CYS	A	575	-7.339	8.014	8.820	1.00	17.32	C
ATOM	1950	CB	CYS	A	575	-6.264	7.728	7.762	1.00	20.93	C
ATOM	1951	SG	CYS	A	575	-6.765	8.124	6.035	1.00	23.46	S
ATOM	1952	C	CYS	A	575	-6.855	7.431	10.156	1.00	21.12	C
ATOM	1953	O	CYS	A	575	-6.857	6.215	10.343	1.00	19.67	O
ATOM	1954	N	TRP	A	576	-6.423	8.322	11.047	1.00	19.86	N
ATOM	1955	CA	TRP	A	576	-5.934	7.931	12.370	1.00	21.52	C
ATOM	1956	CB	TRP	A	576	-4.611	8.626	12.709	1.00	20.08	C
ATOM	1957	CG	TRP	A	576	-3.521	8.406	11.707	1.00	19.69	C
ATOM	1958	CD2	TRP	A	576	-2.500	9.333	11.360	1.00	16.53	C
ATOM	1959	CE2	TRP	A	576	-1.694	8.716	10.367	1.00	18.10	C
ATOM	1960	CE3	TRP	A	576	-2.180	10.634	11.796	1.00	17.50	C
ATOM	1961	CD1	TRP	A	576	-3.312	7.284	10.950	1.00	20.54	C
ATOM	1962	NE1	TRP	A	576	-2.207	7.464	10.137	1.00	18.64	N
ATOM	1963	CZ2	TRP	A	576	-0.584	9.357	9.790	1.00	20.52	C
ATOM	1964	CZ3	TRP	A	576	-1.064	11.282	11.231	1.00	19.63	C
ATOM	1965	CH2	TRP	A	576	-0.280	10.638	10.231	1.00	18.57	C
ATOM	1966	C	TRP	A	576	-6.914	8.185	13.520	1.00	21.81	C
ATOM	1967	O	TRP	A	576	-6.487	8.424	14.664	1.00	21.51	O
ATOM	1968	N	ILE	A	577	-8.211	8.166	13.200	1.00	19.65	N
ATOM	1969	CA	ILE	A	577	-9.247	8.325	14.224	1.00	20.80	C
ATOM	1970	CB	ILE	A	577	-10.637	8.526	13.566	1.00	22.18	C
ATOM	1971	CG2	ILE	A	577	-11.783	8.179	14.574	1.00	20.80	C
ATOM	1972	CG1	ILE	A	577	-10.749	9.997	13.091	1.00	27.26	C
ATOM·	1973	CD1	ILE	A	577	-11.997	10.298	12.254	1.00	29.41	C
ATOM	1974	C	ILE	A	577	-9.194	7.014	15.029	1.00	18.87	C
ATOM	1975	O	ILE	A	577	-9.204	5.927	14.455	1.00	21.86	O
ATOM	1976	N	TYR	A	578	-9.099	7.143	16.349	1.00	20.88	N
ATOM	1977	CA	TYR	A	578	-8.958	5.973	17.210	1.00	25.32	C
ATOM	1978	CB	TYR	A	578	-8.815	6.429	18.672	1.00	23.94	C
ATOM	1979	CG	TYR	A	578	-8.350	5.327	19.619	1.00	26.11	C
ATOM	1980	CD1	TYR	A	578	-7.000	5.188	19.946	1.00	31.42	C
ATOM	1981	CE1	TYR	A	578	-6.561	4.141	20.787	1.00	32.15	C
ATOM	1982	CD2	TYR	A	578	-9.256	4.401	20.158	1.00	33.33	C
ATOM	1983	CE2	TYR	A	578	-8.820	3.354	20.991	1.00	33.06	C
ATOM	1984	CZ	TYR	A	578	-7.468	3.232	21.295	1.00	31.77	C
ATOM	1985	OH	TYR	A	578	-7.016	2.178	22.088	1.00	33.01	O
ATOM	1986	C	TYR	A	578	-10.080	4.947	17.108	1.00	27.02	C
ATOM	1987	O	TYR	A	578	-9.819	3.750	16.903	1.00	22.11	O
ATOM	1988	N	LYS	A	579	-11.313	5.418	17.310	1.00	24.58	N
ATOM	1989	CA	LYS	A	579	-12.500	4.583	17.290	1.00	27.83	C
ATOM	1990	CB	LYS	A	579	-13.727	5.372	17.776	1.00	29.76	C
ATOM	1991	CG	LYS	A	579	-13.639	5.869	19.229	1.00	39.10	C
ATOM	1992	CD	LYS	A	579	-14.979	6.478	19.709	1.00	42.19	C
ATOM	1993	CE	LYS	A	579	-14.918	6.879	21.192	1.00	50.93	C
ATOM	1994	NZ	LYS	A	579	-16.124	7.694	21.593	1.00	50.31	N
ATOM	1995	C	LYS	A	579	-12.774	4.050	15.904	1.00	29.39	C
ATOM	1996	O	LYS	A	579	-12.998	4.803	14.976	1.00	27.65	O
ATOM	1997	N	TRP	A	580	-12.772	2.729	15.802	1.00	26.39	N
ATOM	1998	CA	TRP	A	580	-13.012	2.038	14.544	1.00	31.72	C
ATOM	1999	CB	TRP	A	580	-13.087	0.542	14.847	1.00	33.80	C
ATOM	2000	CG	TRP	A	580	-13.287	-0.297	13.670	1.00	36.87	C
ATOM	2001	CD2	TRP	A	580	-14.500	-0.948	13.288	1.00	37.12	C
ATOM	2002	CE2	TRP	A	580	-14.230	-1.666	12.097	1.00	42.38	C
ATOM	2003	CE3	TRP	A	580	-15.792	-0.998	13.835	1.00	43.97	C

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ATOM   2004  CD1 TRP A 580    -12.355   -0.624   12.728  1.00 41.08        C
ATOM   2005  NE1 TRP A 580    -12.915   -1.452   11.777  1.00 37.64        N
ATOM   2006  CZ2 TRP A 580    -15.205   -2.428   11.440  1.00 40.07        C
ATOM   2007  CZ3 TRP A 580    -16.766   -1.757   13.182  1.00 45.16        C
ATOM   2008  CH2 TRP A 580    -16.464   -2.462   11.996  1.00 48.53        C
ATOM   2009  C   TRP A 580    -14.297    2.492   13.847  1.00 32.01        C
ATOM   2010  O   TRP A 580    -14.300    2.806   12.651  1.00 29.01        O
ATOM   2011  N   GLU A 581    -15.395    2.528   14.590  1.00 26.90        N
ATOM   2012  CA  GLU A 581    -16.673    2.930   14.006  1.00 31.38        C
ATOM   2013  CB  GLU A 581    -17.785    2.761   15.043  1.00 42.49        C
ATOM   2014  CG  GLU A 581    -17.518    1.642   16.043  1.00 44.23        C
ATOM   2015  CD  GLU A 581    -16.725    2.134   17.243  1.00 54.00        C
ATOM   2016  OE1 GLU A 581    -17.263    2.985   17.997  1.00 62.87        O
ATOM   2017  OE2 GLU A 581    -15.576    1.686   17.440  1.00 44.35        O
ATOM   2018  C   GLU A 581    -16.703    4.365   13.461  1.00 31.42        C
ATOM   2019  O   GLU A 581    -17.501    4.671   12.585  1.00 32.84        O
ATOM   2020  N   ASP A 582    -15.824    5.232   13.963  1.00 29.31        N
ATOM   2021  CA  ASP A 582    -15.779    6.631   13.543  1.00 26.27        C
ATOM   2022  CB  ASP A 582    -15.502    7.525   14.759  1.00 30.65        C
ATOM   2023  CG  ASP A 582    -16.611    7.449   15.799  1.00 38.03        C
ATOM   2024  OD1 ASP A 582    -17.741    7.089   15.416  1.00 34.32        O
ATOM   2025  OD2 ASP A 582    -16.357    7.744   16.989  1.00 35.77        O
ATOM   2026  C   ASP A 582    -14.741    6.955   12.458  1.00 28.97        C
ATOM   2027  O   ASP A 582    -14.682    8.086   11.957  1.00 25.58        O
ATOM   2028  N   ARG A 583    -13.926    5.970   12.107  1.00 26.36        N
ATOM   2029  CA  ARG A 583    -12.883    6.195   11.108  1.00 26.57        C
ATOM   2030  CB  ARG A 583    -11.756    5.153   11.313  1.00 24.45        C
ATOM   2031  CG  ARG A 583    -10.396    5.437   10.597  1.00 21.69        C
ATOM   2032  CD  ARG A 583     -9.414    4.259   10.869  1.00 18.39        C
ATOM   2033  NE  ARG A 583     -9.289    4.015   12.315  1.00 17.34        N
ATOM   2034  CZ  ARG A 583     -9.081    2.825   12.866  1.00 21.68        C
ATOM   2035  NH1 ARG A 583     -8.963    1.744   12.113  1.00 18.82        N
ATOM   2036  NH2 ARG A 583     -9.029    2.717   14.200  1.00 22.38        N
ATOM   2037  C   ARG A 583    -13.525    6.070    9.720  1.00 24.67        C
ATOM   2038  O   ARG A 583    -14.382    5.223    9.485  1.00 25.78        O
ATOM   2039  N   PRO A 584    -13.109    6.916    8.769  1.00 23.39        N
ATOM   2040  CD  PRO A 584    -12.146    8.027    8.893  1.00 25.28        C
ATOM   2041  CA  PRO A 584    -13.667    6.869    7.407  1.00 25.72        C
ATOM   2042  CB  PRO A 584    -13.073    8.097    6.736  1.00 26.27        C
ATOM   2043  CG  PRO A 584    -11.760    8.276    7.437  1.00 22.96        C
ATOM   2044  C   PRO A 584    -13.318    5.609    6.620  1.00 26.41        C
ATOM   2045  O   PRO A 584    -12.329    4.940    6.930  1.00 23.65        O
ATOM   2046  N   ASP A 585    -14.142    5.313    5.610  1.00 20.71        N
ATOM   2047  CA  ASP A 585    -13.920    4.182    4.714  1.00 20.68        C
ATOM   2048  CB  ASP A 585    -15.258    3.578    4.236  1.00 31.23        C
ATOM   2049  CG  ASP A 585    -16.100    3.042    5.380  1.00 41.40        C
ATOM   2050  OD1 ASP A 585    -15.581    2.249    6.197  1.00 48.33        O
ATOM   2051  OD2 ASP A 585    -17.295    3.419    5.453  1.00 55.79        O
ATOM   2052  C   ASP A 585    -13.183    4.695    3.471  1.00 19.99        C
ATOM   2053  O   ASP A 585    -13.097    5.907    3.256  1.00 24.11        O
ATOM   2054  N   PHE A 586    -12.692    3.777    2.636  1.00 21.55        N
ATOM   2055  CA  PHE A 586    -11.960    4.193    1.439  1.00 25.44        C
ATOM   2056  CB  PHE A 586    -11.231    3.013    0.780  1.00 23.78        C
ATOM   2057  CG  PHE A 586     -9.909    2.689    1.445  1.00 21.80        C
ATOM   2058  CD1 PHE A 586     -8.837    3.578    1.392  1.00 26.67        C
ATOM   2059  CD2 PHE A 586     -9.754    1.480    2.146  1.00 26.93        C
ATOM   2060  CE1 PHE A 586     -7.606    3.261    2.026  1.00 19.00        C
ATOM   2061  CE2 PHE A 586     -8.546    1.175    2.767  1.00 22.77        C
ATOM   2062  CZ  PHE A 586     -7.482    2.056    2.701  1.00 20.88        C
ATOM   2063  C   PHE A 586    -12.863    4.894    0.430  1.00 25.78        C
ATOM   2064  O   PHE A 586    -12.399    5.669   -0.358  1.00 22.13        O
ATOM   2065  N   LEU A 587    -14.168    4.628    0.487  1.00 27.35        N
ATOM   2066  CA  LEU A 587    -15.082    5.342   -0.410  1.00 27.54        C
ATOM   2067  CB  LEU A 587    -16.525    4.916   -0.107  1.00 33.35        C
ATOM   2068  CG  LEU A 587    -17.649    5.418   -1.010  1.00 40.50        C
ATOM   2069  CD1 LEU A 587    -17.775    6.902   -0.854  1.00 43.82        C
ATOM   2070  CD2 LEU A 587    -17.358    5.069   -2.455  1.00 41.16        C
ATOM   2071  C   LEU A 587    -14.879    6.856   -0.178  1.00 21.74        C
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ATOM	2072	O	LEU	A	587	-14.638	7.596	-1.137	1.00	29.01	O
ATOM	2073	N	THR	A	588	-14.923	7.322	1.077	1.00	21.57	N
ATOM	2074	CA	THR	A	588	-14.718	8.743	1.326	1.00	25.49	C
ATOM	2075	CB	THR	A	588	-15.271	9.205	2.705	1.00	35.32	C
ATOM	2076	OG1	THR	A	588	-14.462	8.694	3.759	1.00	46.78	O
ATOM	2077	CG2	THR	A	588	-16.687	8.707	2.879	1.00	33.61	C
ATOM	2078	C	THR	A	588	-13.257	9.153	1.212	1.00	28.40	C
ATOM	2079	O	THR	A	588	-12.964	10.229	0.705	1.00	26.45	O
ATOM	2080	N	VAL	A	589	-12.341	8.293	1.670	1.00	22.28	N
ATOM	2081	CA	VAL	A	589	-10.927	8.646	1.549	1.00	19.94	C
ATOM	2082	CB	VAL	A	589	-10.021	7.525	2.161	1.00	27.25	C
ATOM	2083	CG1	VAL	A	589	-8.539	7.770	1.790	1.00	22.69	C
ATOM	2084	CG2	VAL	A	589	-10.180	7.525	3.673	1.00	24.26	C
ATOM	2085	C	VAL	A	589	-10.502	8.911	0.102	1.00	20.96	C
ATOM	2086	O	VAL	A	589	-9.788	9.888	-0.178	1.00	21.66	O
ATOM	2087	N	GLU	A	590	-10.932	8.047	-0.818	1.00	23.06	N
ATOM	2088	CA	GLU	A	590	-10.583	8.205	-2.227	1.00	22.93	C
ATOM	2089	CB	GLU	A	590	-11.130	7.022	-3.049	1.00	24.91	C
ATOM	2090	CG	GLU	A	590	-10.775	7.021	-4.559	1.00	27.15	C
ATOM	2091	CD	GLU	A	590	-11.603	8.014	-5.414	1.00	31.97	C
ATOM	2092	OE1	GLU	A	590	-12.804	8.214	-5.130	1.00	31.00	O
ATOM	2093	OE2	GLU	A	590	-11.056	8.562	-6.399	1.00	29.57	O
ATOM	2094	C	GLU	A	590	-11.137	9.531	-2.784	1.00	25.86	C
ATOM	2095	O	GLU	A	590	-10.466	10.218	-3.552	1.00	21.69	O
ATOM	2096	N	GLN	A	591	-12.362	9.875	-2.394	1.00	24.00	N
ATOM	2097	CA	GLN	A	591	-12.972	11.131	-2.856	1.00	27.84	C
ATOM	2098	CB	GLN	A	591	-14.426	11.197	-2.398	1.00	29.39	C
ATOM	2099	CG	GLN	A	591	-15.298	10.136	-2.993	1.00	32.75	C
ATOM	2100	CD	GLN	A	591	-16.754	10.334	-2.629	1.00	38.78	C
ATOM	2101	OE1	GLN	A	591	-17.078	11.132	-1.745	1.00	43.77	O
ATOM	2102	NE2	GLN	A	591	-17.636	9.614	-3.302	1.00	44.60	N
ATOM	2103	C	GLN	A	591	-12.240	12.361	-2.354	1.00	28.08	C
ATOM	2104	O	GLN	A	591	-12.023	13.332	-3.097	1.00	27.52	O
ATOM	2105	N	ARG	A	592	-11.851	12.345	-1.084	1.00	24.43	N
ATOM	2106	CA	ARG	A	592	-11.138	13.471	-0.520	1.00	25.06	C
ATOM	2107	CB	ARG	A	592	-11.060	13.338	1.004	1.00	25.79	C
ATOM	2108	CG	ARG	A	592	-12.433	13.494	1.649	1.00	28.74	C
ATOM	2109	CD	ARG	A	592	-12.418	13.215	3.127	1.00	31.24	C
ATOM	2110	NE	ARG	A	592	-11.576	14.162	3.844	1.00	25.60	N
ATOM	2111	CZ	ARG	A	592	-11.336	14.096	5.146	1.00	25.97	C
ATOM	2112	NH1	ARG	A	592	-11.883	13.123	5.859	1.00	27.29	N
ATOM	2113	NH2	ARG	A	592	-10.551	14.996	5.720	1.00	28.63	N
ATOM	2114	C	ARG	A	592	-9.750	13.563	-1.117	1.00	25.17	C
ATOM	2115	O	ARG	A	592	-9.235	14.667	-1.360	1.00	26.90	O
ATOM	2116	N	MET	A	593	-9.138	12.409	-1.368	1.00	23.69	N
ATOM	2117	CA	MET	A	593	-7.796	12.416	-1.931	1.00	28.31	C
ATOM	2118	CB	MET	A	593	-7.192	11.000	-1.892	1.00	23.46	C
ATOM	2119	CG	MET	A	593	-5.743	10.934	-2.292	1.00	23.72	C
ATOM	2120	SD	MET	A	593	-4.646	11.896	-1.177	1.00	28.98	S
ATOM	2121	CE	MET	A	593	-3.866	12.944	-2.359	1.00	26.58	C
ATOM	2122	C	MET	A	593	-7.862	12.937	-3.372	1.00	26.14	C
ATOM	2123	O	MET	A	593	-6.998	13.697	-3.802	1.00	28.83	O
ATOM	2124	N	ARG	A	594	-8.877	12.519	-4.117	1.00	23.87	N
ATOM	2125	CA	ARG	A	594	-9.023	12.958	-5.498	1.00	24.90	C
ATOM	2126	CB	ARG	A	594	-10.275	12.328	-6.106	1.00	21.24	C
ATOM	2127	CG	ARG	A	594	-10.482	12.694	-7.596	1.00	25.80	C
ATOM	2128	CD	ARG	A	594	-11.817	12.169	-8.118	1.00	36.37	C
ATOM	2129	NE	ARG	A	594	-11.832	10.715	-8.236	1.00	43.01	N
ATOM	2130	CZ	ARG	A	594	-11.353	10.041	-9.281	1.00	44.29	C
ATOM	2131	NH1	ARG	A	594	-10.823	10.690	-10.313	1.00	45.97	N
ATOM	2132	NH2	ARG	A	594	-11.387	8.716	-9.289	1.00	38.74	N
ATOM	2133	C	ARG	A	594	-9.116	14.494	-5.542	1.00	28.27	C
ATOM	2134	O	ARG	A	594	-8.465	15.150	-6.362	1.00	30.97	O
ATOM	2135	N	ALA	A	595	-9.911	15.050	-4.637	1.00	30.31	N
ATOM	2136	CA	ALA	A	595	-10.118	16.495	-4.530	1.00	34.21	C
ATOM	2137	CB	ALA	A	595	-11.224	16.787	-3.496	1.00	32.96	C
ATOM	2138	C	ALA	A	595	-8.834	17.234	-4.161	1.00	36.64	C
ATOM	2139	O	ALA	A	595	-8.550	18.300	-4.705	1.00	34.21	O

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ATOM	2140	N	CYS	A	596	-8.057	16.664	-3.237	1.00	31.92	N
ATOM	2141	CA	CYS	A	596	-6.803	17.277	-2.826	1.00	33.56	C
ATOM	2142	CB	CYS	A	596	-6.169	16.505	-1.655	1.00	31.86	C
ATOM	2143	SG	CYS	A	596	-7.012	16.710	-0.074	1.00	40.76	S
ATOM	2144	C	CYS	A	596	-5.830	17.280	-3.990	1.00	32.72	C
ATOM	2145	O	CYS	A	596	-5.155	18.279	-4.245	1.00	31.91	O
ATOM	2146	N	TYR	A	597	-5.747	16.150	-4.686	1.00	28.25	N
ATOM	2147	CA	TYR	A	597	-4.832	16.036	-5.814	1.00	30.48	C
ATOM	2148	CB	TYR	A	597	-4.881	14.615	-6.389	1.00	31.14	C
ATOM	2149	CG	TYR	A	597	-4.225	14.464	-7.742	1.00	31.11	C
ATOM	2150	CD1	TYR	A	597	-2.963	15.000	-7.993	1.00	32.87	C
ATOM	2151	CE1	TYR	A	597	-2.370	14.894	-9.259	1.00	37.85	C
ATOM	2152	CD2	TYR	A	597	-4.877	13.806	-8.780	1.00	34.93	C
ATOM	2153	CE2	TYR	A	597	-4.298	13.687	-10.047	1.00	41.03	C
ATOM	2154	CZ	TYR	A	597	-3.048	14.240	-10.281	1.00	39.13	C
ATOM	2155	OH	TYR	A	597	-2.505	14.165	-11.543	1.00	39.42	O
ATOM	2156	C	TYR	A	597	-5.168	17.049	-6.907	1.00	34.57	C
ATOM	2157	O	TYR	A	597	-4.275	17.751	-7.421	1.00	33.33	O
ATOM	2158	N	TYR	A	598	-6.446	17.106	-7.261	1.00	30.49	N
ATOM	2159	CA	TYR	A	598	-6.921	18.019	-8.298	1.00	40.96	C
ATOM	2160	CB	TYR	A	598	-8.427	17.833	-8.532	1.00	38.84	C
ATOM	2161	CG	TYR	A	598	-8.800	16.590	-9.316	1.00	41.02	C
ATOM	2162	CD1	TYR	A	598	-10.130	16.335	-9.659	1.00	49.62	C
ATOM	2163	CE1	TYR	A	598	-10.490	15.170	-10.353	1.00	49.11	C
ATOM	2164	CD2	TYR	A	598	-7.838	15.651	-9.691	1.00	46.14	C
ATOM	2165	CE2	TYR	A	598	-8.182	14.489	-10.377	1.00	45.32	C
ATOM	2166	CZ	TYR	A	598	-9.511	14.252	-10.703	1.00	50.82	C
ATOM	2167	OH	TYR	A	598	-9.857	13.082	-11.342	1.00	48.64	O
ATOM	2168	C	TYR	A	598	-6.630	19.453	-7.903	1.00	44.26	C
ATOM	2169	O	TYR	A	598	-6.255	20.275	-8.744	1.00	50.25	O
ATOM	2170	N	SER	A	599	-6.790	19.759	-6.623	1.00	36.48	N
ATOM	2171	CA	SER	A	599	-6.525	21.095	-6.132	1.00	42.68	C
ATOM	2172	CB	SER	A	599	-6.935	21.185	-4.670	1.00	43.70	C
ATOM	2173	OG	SER	A	599	-6.732	22.487	-4.171	1.00	57.23	O
ATOM	2174	C	SER	A	599	-5.035	21.427	-6.295	1.00	46.61	C
ATOM	2175	O	SER	A	599	-4.663	22.541	-6.686	1.00	38.28	O
ATOM	2176	N	LEU	A	600	-4.176	20.459	-6.006	1.00	35.37	N
ATOM	2177	CA	LEU	A	600	-2.740	20.681	-6.137	1.00	43.98	C
ATOM	2178	CB	LEU	A	600	-1.955	19.613	-5.372	1.00	36.49	C
ATOM	2179	CG	LEU	A	600	-2.119	19.658	-3.850	1.00	42.50	C
ATOM	2180	CD1	LEU	A	600	-1.522	18.409	-3.229	1.00	35.50	C
ATOM	2181	CD2	LEU	A	600	-1.449	20.896	-3.293	1.00	45.68	C
ATOM	2182	C	LEU	A	600	-2.301	20.674	-7.587	1.00	41.54	C
ATOM	2183	O	LEU	A	600	-1.381	21.406	-7.965	1.00	46.25	O
ATOM	2184	N	ALA	A	601	-2.963	19.850	-8.393	1.00	38.74	N
ATOM	2185	CA	ALA	A	601	-2.648	19.698	-9.811	1.00	47.05	C
ATOM	2186	CB	ALA	A	601	-3.470	18.564	-10.404	1.00	45.68	C
ATOM	2187	C	ALA	A	601	-2.912	20.997	-10.569	1.00	52.87	C
ATOM	2188	O	ALA	A	601	-2.239	21.306	-11.556	1.00	53.37	O
ATOM	2189	N	SER	A	602	-3.899	21.748	-10.094	1.00	51.50	N
ATOM	2190	CA	SER	A	602	-4.266	23.024	-10.691	1.00	57.64	C
ATOM	2191	CB	SER	A	602	-5.750	23.293	-10.458	1.00	57.42	C
ATOM	2192	OG	SER	A	602	-6.542	22.301	-11.091	1.00	55.95	O
ATOM	2193	C	SER	A	602	-3.428	24.130	-10.054	1.00	59.56	C
ATOM	2194	O	SER	A	602	-3.790	25.302	-10.103	1.00	64.84	O
ATOM	2195	N	LYS	A	603	-2.307	23.730	-9.459	1.00	63.84	N
ATOM	2196	CA	LYS	A	603	-1.378	24.639	-8.792	1.00	65.05	C
ATOM	2197	CB	LYS	A	603	-0.968	25.767	-9.747	1.00	65.01	C
ATOM	2198	CG	LYS	A	603	0.509	26.120	-9.697	1.00	65.21	C
ATOM	2199	CD	LYS	A	603	0.835	27.209	-10.706	1.00	65.84	C
ATOM	2200	CE	LYS	A	603	2.334	27.480	-10.766	1.00	67.72	C
ATOM	2201	NZ	LYS	A	603	2.656	28.634	-11.659	1.00	67.84	N
ATOM	2202	C	LYS	A	603	-2.011	25.214	-7.519	1.00	65.66	C
ATOM	2203	O	LYS	A	603	-1.435	25.016	-6.424	1.00	67.21	O
ATOM	2204	OXT	LYS	A	603	-3.085	25.847	-7.626	1.00	69.14	O
TER	1		LYS	A	603						
ATOM	2205	CB	PHE	B	331	26.385	4.944	44.783	1.00	47.38	C
ATOM	2206	CG	PHE	B	331	26.386	4.527	43.338	1.00	47.76	C

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ATOM	2207	CD1	PHE	B	331	27.574	4.465	42.621	1.00	52.74	C
ATOM	2208	CD2	PHE	B	331	25.201	4.218	42.689	1.00	47.87	C
ATOM	2209	CE1	PHE	B	331	27.582	4.104	41.283	1.00	48.41	C
ATOM	2210	CE2	PHE	B	331	25.196	3.855	41.347	1.00	52.09	C
ATOM	2211	CZ	PHE	B	331	26.387	3.797	40.643	1.00	50.05	C
ATOM	2212	C	PHE	B	331	26.230	6.878	46.363	1.00	45.38	C
ATOM	2213	O	PHE	B	331	27.005	6.988	47.313	1.00	49.66	O
ATOM	2214	N	PHE	B	331	28.209	6.632	44.860	1.00	48.36	N
ATOM	2215	CA	PHE	B	331	26.733	6.417	44.999	1.00	44.38	C
ATOM	2216	N	LEU	B	332	24.933	7.156	46.441	1.00	39.16	N
ATOM	2217	CA	LEU	B	332	24.306	7.623	47.678	1.00	40.71	C
ATOM	2218	CB	LEU	B	332	23.601	8.967	47.426	1.00	40.95	C
ATOM	2219	CG	LEU	B	332	24.412	10.129	46.828	1.00	42.67	C
ATOM	2220	CD1	LEU	B	332	23.451	11.230	46.342	1.00	38.80	C
ATOM	2221	CD2	LEU	B	332	25.394	10.684	47.864	1.00	39.78	C
ATOM	2222	C	LEU	B	332	23.276	6.592	48.138	1.00	42.07	C
ATOM	2223	O	LEU	B	332	22.808	5.781	47.347	1.00	39.83	O
ATOM	2224	N	LYS	B	333	22.929	6.621	49.423	1.00	42.54	N
ATOM	2225	CA	LYS	B	333	21.927	5.699	49.947	1.00	44.61	C
ATOM	2226	CB	LYS	B	333	22.050	5.571	51.467	1.00	46.09	C
ATOM	2227	CG	LYS	B	333	23.341	4.930	51.902	1.00	50.67	C
ATOM	2228	CD	LYS	B	333	23.230	4.443	53.337	1.00	58.35	C
ATOM	2229	CE	LYS	B	333	24.498	3.707	53.764	1.00	59.84	C
ATOM	2230	NZ	LYS	B	333	24.351	3.125	55.132	1.00	62.41	N
ATOM	2231	C	LYS	B	333	20.542	6.206	49.605	1.00	41.31	C
ATOM	2232	O	LYS	B	333	20.214	7.357	49.888	1.00	39.53	O
ATOM	2233	N	ARG	B	334	19.729	5.332	49.021	1.00	36.95	N
ATOM	2234	CA	ARG	B	334	18.375	5.682	48.628	1.00	43.46	C
ATOM	2235	CB	ARG	B	334	17.707	4.487	47.944	1.00	44.85	C
ATOM	2236	CG	ARG	B	334	16.275	4.735	47.485	1.00	43.32	C
ATOM	2237	CD	ARG	B	334	16.238	5.676	46.299	1.00	38.79	C
ATOM	2238	NE	ARG	B	334	14.873	5.974	45.879	1.00	37.97	N
ATOM	2239	CZ	ARG	B	334	14.074	6.819	46.509	1.00	38.57	C
ATOM	2240	NH1	ARG	B	334	14.505	7.457	47.595	1.00	36.94	N
ATOM	2241	NH2	ARG	B	334	12.846	7.038	46.054	1.00	42.39	N
ATOM	2242	C	ARG	B	334	17.547	6.103	49.839	1.00	45.57	C
ATOM	2243	O	ARG	B	334	16.571	6.845	49.712	1.00	41.28	O
ATOM	2244	N	ASP	B	335	17.960	5.619	51.010	1.00	46.31	N
ATOM	2245	CA	ASP	B	335	17.274	5.898	52.272	1.00	45.57	C
ATOM	2246	CB	ASP	B	335	17.823	4.969	53.354	1.00	51.22	C
ATOM	2247	CG	ASP	B	335	17.911	3.533	52.887	1.00	54.98	C
ATOM	2248	OD1	ASP	B	335	16.856	2.869	52.816	1.00	60.53	O
ATOM	2249	OD2	ASP	B	335	19.032	3.074	52.567	1.00	62.94	O
ATOM	2250	C	ASP	B	335	17.439	7.338	52.719	1.00	42.46	C
ATOM	2251	O	ASP	B	335	16.647	7.840	53.525	1.00	36.68	O
ATOM	2252	N	ASN	B	336	18.471	8.010	52.219	1.00	29.28	N
ATOM	2253	CA	ASN	B	336	18.713	9.383	52.603	1.00	31.89	C
ATOM	2254	CB	ASN	B	336	20.211	9.667	52.652	1.00	33.88	C
ATOM	2255	CG	ASN	B	336	20.904	8.875	53.734	1.00	49.73	C
ATOM	2256	OD1	ASN	B	336	20.356	8.676	54.822	1.00	46.67	O
ATOM	2257	ND2	ASN	B	336	22.124	8.437	53.452	1.00	47.83	N
ATOM	2258	C	ASN	B	336	18.054	10.366	51.655	1.00	27.35	C
ATOM	2259	O	ASN	B	336	18.188	11.571	51.819	1.00	28.55	O
ATOM	2260	N	LEU	B	337	17.341	9.834	50.679	1.00	31.14	N
ATOM	2261	CA	LEU	B	337	16.687	10.667	49.677	1.00	34.02	C
ATOM	2262	CB	LEU	B	337	17.174	10.263	48.277	1.00	30.37	C
ATOM	2263	CG	LEU	B	337	16.623	11.013	47.049	1.00	29.39	C
ATOM	2264	CD1	LEU	B	337	17.255	12.379	46.971	1.00	29.26	C
ATOM	2265	CD2	LEU	B	337	16.949	10.246	45.775	1.00	35.80	C
ATOM	2266	C	LEU	B	337	15.163	10.583	49.728	1.00	29.91	C
ATOM	2267	O	LEU	B	337	14.581	9.510	49.799	1.00	30.87	O
ATOM	2268	N	LEU	B	338	14.516	11.733	49.674	1.00	26.54	N
ATOM	2269	CA	LEU	B	338	13.060	11.780	49.667	1.00	26.34	C
ATOM	2270	CB	LEU	B	338	12.534	12.524	50.910	1.00	27.85	C
ATOM	2271	CG	LEU	B	338	10.999	12.521	51.023	1.00	29.64	C
ATOM	2272	CD1	LEU	B	338	10.508	11.097	51.215	1.00	34.52	C
ATOM	2273	CD2	LEU	B	338	10.550	13.388	52.184	1.00	29.92	C
ATOM	2274	C	LEU	B	338	12.693	12.562	48.397	1.00	29.11	C

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ATOM   2275  O    LEU B 338     12.941  13.762  48.321  1.00  29.08           O
ATOM   2276  N    ILE B 339     12.145  11.868  47.402  1.00  29.57           N
ATOM   2277  CA   ILE B 339     11.785  12.534  46.150  1.00  28.48           C
ATOM   2278  CB   ILE B 339     11.902  11.564  44.950  1.00  32.66           C
ATOM   2279  CG2  ILE B 339     11.633  12.331  43.627  1.00  32.51           C
ATOM   2280  CG1  ILE B 339     13.286  10.909  44.961  1.00  32.18           C
ATOM   2281  CD1  ILE B 339     13.495   9.849  43.902  1.00  41.01           C
ATOM   2282  C    ILE B 339     10.366  13.062  46.208  1.00  31.19           C
ATOM   2283  O    ILE B 339      9.431  12.309  46.466  1.00  33.54           O
ATOM   2284  N    ALA B 340     10.208  14.358  45.965  1.00  28.66           N
ATOM   2285  CA   ALA B 340      8.880  14.966  45.989  1.00  34.20           C
ATOM   2286  CB   ALA B 340      8.990  16.462  46.265  1.00  32.40           C
ATOM   2287  C    ALA B 340      8.152  14.717  44.667  1.00  36.35           C
ATOM   2288  O    ALA B 340      8.775  14.336  43.663  1.00  35.42           O
ATOM   2289  N    ASP B 341      6.836  14.907  44.674  1.00  33.98           N
ATOM   2290  CA   ASP B 341      6.041  14.711  43.469  1.00  39.65           C
ATOM   2291  CB   ASP B 341      4.631  14.226  43.840  1.00  45.61           C
ATOM   2292  CG   ASP B 341      3.912  13.554  42.670  1.00  57.27           C
ATOM   2293  OD1  ASP B 341      4.096  14.002  41.519  1.00  59.44           O
ATOM   2294  OD2  ASP B 341      3.149  12.582  42.901  1.00  63.51           O
ATOM   2295  C    ASP B 341      5.959  16.070  42.779  1.00  44.29           C
ATOM   2296  O    ASP B 341      4.868  16.568  42.502  1.00  45.33           O
ATOM   2297  N    ILE B 342      7.119  16.671  42.514  1.00  36.54           N
ATOM   2298  CA   ILE B 342      7.202  17.981  41.879  1.00  36.97           C
ATOM   2299  CB   ILE B 342      7.661  19.043  42.896  1.00  38.63           C
ATOM   2300  CG2  ILE B 342      7.852  20.397  42.215  1.00  42.84           C
ATOM   2301  CG1  ILE B 342      6.645  19.131  44.033  1.00  39.67           C
ATOM   2302  CD1  ILE B 342      7.093  20.032  45.166  1.00  46.12           C
ATOM   2303  C    ILE B 342      8.225  17.899  40.753  1.00  37.86           C
ATOM   2304  O    ILE B 342      9.336  17.438  40.961  1.00  33.45           O
ATOM   2305  N    GLU B 343      7.840  18.335  39.561  1.00  31.27           N
ATOM   2306  CA   GLU B 343      8.736  18.281  38.415  1.00  35.65           C
ATOM   2307  CB   GLU B 343      7.994  17.733  37.194  1.00  35.13           C
ATOM   2308  CG   GLU B 343      8.842  17.680  35.940  1.00  40.36           C
ATOM   2309  CD   GLU B 343      8.204  16.874  34.824  1.00  49.77           C
ATOM   2310  OE1  GLU B 343      8.173  15.627  34.926  1.00  48.98           O
ATOM   2311  OE2  GLU B 343      7.734  17.488  33.845  1.00  50.13           O
ATOM   2312  C    GLU B 343      9.287  19.661  38.112  1.00  35.92           C
ATOM   2313  O    GLU B 343      8.522  20.568  37.825  1.00  33.14           O
ATOM   2314  N    LEU B 344     10.612  19.811  38.179  1.00  26.19           N
ATOM   2315  CA   LEU B 344     11.245  21.100  37.907  1.00  26.71           C
ATOM   2316  CB   LEU B 344     12.646  21.179  38.577  1.00  25.66           C
ATOM   2317  CG   LEU B 344     12.593  21.025  40.097  1.00  30.64           C
ATOM   2318  CD1  LEU B 344     14.017  20.874  40.644  1.00  27.22           C
ATOM   2319  CD2  LEU B 344     11.877  22.223  40.737  1.00  33.34           C
ATOM   2320  C    LEU B 344     11.373  21.299  36.404  1.00  25.27           C
ATOM   2321  O    LEU B 344     11.313  22.428  35.912  1.00  30.00           O
ATOM   2322  N    GLY B 345     11.576  20.206  35.672  1.00  24.88           N
ATOM   2323  CA   GLY B 345     11.683  20.297  34.228  1.00  29.60           C
ATOM   2324  C    GLY B 345     11.779  18.915  33.635  1.00  29.46           C
ATOM   2325  O    GLY B 345     11.720  17.929  34.366  1.00  32.49           O
ATOM   2326  N    CYS B 346     11.915  18.818  32.315  1.00  27.20           N
ATOM   2327  CA   CYS B 346     12.057  17.510  31.688  1.00  32.81           C
ATOM   2328  CB   CYS B 346     10.690  16.909  31.391  1.00  41.74           C
ATOM   2329  SG   CYS B 346      9.815  17.890  30.185  1.00  44.47           S
ATOM   2330  C    CYS B 346     12.843  17.626  30.391  1.00  38.59           C
ATOM   2331  O    CYS B 346     13.184  18.728  29.963  1.00  36.63           O
ATOM   2332  N    GLY B 347     13.120  16.478  29.785  1.00  36.78           N
ATOM   2333  CA   GLY B 347     13.846  16.426  28.528  1.00  36.32           C
ATOM   2334  C    GLY B 347     13.632  15.050  27.936  1.00  37.34           C
ATOM   2335  O    GLY B 347     12.888  14.252  28.505  1.00  35.37           O
ATOM   2336  N    ASN B 348     14.274  14.760  26.812  1.00  38.30           N
ATOM   2337  CA   ASN B 348     14.143  13.451  26.180  1.00  41.78           C
ATOM   2338  CB   ASN B 348     14.905  13.414  24.850  1.00  50.03           C
ATOM   2339  CG   ASN B 348     14.269  14.284  23.799  1.00  55.15           C
ATOM   2340  OD1  ASN B 348     13.105  14.090  23.440  1.00  59.57           O
ATOM   2341  ND2  ASN B 348     15.028  15.256  23.289  1.00  59.33           N
ATOM   2342  C    ASN B 348     14.670  12.334  27.077  1.00  39.62           C
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ATOM   2343  O   ASN B 348     14.281  11.183  26.930  1.00 38.79           O
ATOM   2344  N   PHE B 349     15.565  12.683  28.002  1.00 34.25           N
ATOM   2345  CA  PHE B 349     16.144  11.700  28.915  1.00 36.33           C
ATOM   2346  CB  PHE B 349     17.408  12.277  29.580  1.00 38.59           C
ATOM   2347  CG  PHE B 349     17.140  13.471  30.459  1.00 35.63           C
ATOM   2348  CD1 PHE B 349     16.529  13.315  31.702  1.00 37.36           C
ATOM   2349  CD2 PHE B 349     17.441  14.759  30.022  1.00 35.00           C
ATOM   2350  CE1 PHE B 349     16.216  14.431  32.496  1.00 36.08           C
ATOM   2351  CE2 PHE B 349     17.135  15.872  30.805  1.00 39.51           C
ATOM   2352  CZ  PHE B 349     16.518  15.707  32.047  1.00 34.21           C
ATOM   2353  C   PHE B 349     15.156  11.303  30.014  1.00 34.30           C
ATOM   2354  O   PHE B 349     15.219  10.212  30.562  1.00 37.30           O
ATOM   2355  N   GLY B 350     14.263  12.220  30.358  1.00 34.85           N
ATOM   2356  CA  GLY B 350     13.316  11.949  31.422  1.00 32.42           C
ATOM   2357  C   GLY B 350     12.919  13.235  32.096  1.00 33.80           C
ATOM   2358  O   GLY B 350     12.575  14.204  31.433  1.00 38.01           O
ATOM   2359  N   SER B 351     12.954  13.274  33.421  1.00 34.81           N
ATOM   2360  CA  SER B 351     12.560  14.497  34.079  1.00 31.64           C
ATOM   2361  CB  SER B 351     11.114  14.395  34.536  1.00 42.24           C
ATOM   2362  OG  SER B 351     10.994  13.473  35.583  1.00 38.56           O
ATOM   2363  C   SER B 351     13.461  14.859  35.246  1.00 24.48           C
ATOM   2364  O   SER B 351     14.303  14.076  35.670  1.00 31.02           O
ATOM   2365  N   VAL B 352     13.276  16.064  35.751  1.00 23.21           N
ATOM   2366  CA  VAL B 352     14.069  16.551  36.869  1.00 25.51           C
ATOM   2367  CB  VAL B 352     14.776  17.865  36.521  1.00 23.36           C
ATOM   2368  CG1 VAL B 352     15.570  18.356  37.728  1.00 28.15           C
ATOM   2369  CG2 VAL B 352     15.710  17.645  35.316  1.00 25.42           C
ATOM   2370  C   VAL B 352     13.051  16.809  37.964  1.00 25.74           C
ATOM   2371  O   VAL B 352     12.153  17.661  37.818  1.00 26.16           O
ATOM   2372  N   ARG B 353     13.208  16.078  39.059  1.00 22.97           N
ATOM   2373  CA  ARG B 353     12.299  16.161  40.194  1.00 23.75           C
ATOM   2374  CB  ARG B 353     11.909  14.745  40.652  1.00 25.68           C
ATOM   2375  CG  ARG B 353     11.121  13.891  39.655  1.00 41.51           C
ATOM   2376  CD  ARG B 353      9.703  14.400  39.449  1.00 48.70           C
ATOM   2377  NE  ARG B 353      8.746  13.308  39.273  1.00 58.71           N
ATOM   2378  CZ  ARG B 353      8.258  12.560  40.263  1.00 59.20           C
ATOM   2379  NH1 ARG B 353      8.627  12.776  41.519  1.00 53.03           N
ATOM   2380  NH2 ARG B 353      7.404  11.579  39.992  1.00 59.16           N
ATOM   2381  C   ARG B 353     12.924  16.882  41.366  1.00 29.40           C
ATOM   2382  O   ARG B 353     14.147  16.866  41.554  1.00 30.85           O
ATOM   2383  N   GLN B 354     12.086  17.506  42.178  1.00 26.67           N
ATOM   2384  CA  GLN B 354     12.580  18.193  43.361  1.00 23.26           C
ATOM   2385  CB  GLN B 354     11.648  19.339  43.751  1.00 25.56           C
ATOM   2386  CG  GLN B 354     12.166  20.151  44.923  1.00 30.39           C
ATOM   2387  CD  GLN B 354     11.363  21.415  45.160  1.00 38.39           C
ATOM   2388  OE1 GLN B 354     10.625  21.870  44.288  1.00 35.27           O
ATOM   2389  NE2 GLN B 354     11.523  22.004  46.341  1.00 39.36           N
ATOM   2390  C   GLN B 354     12.589  17.139  44.470  1.00 27.58           C
ATOM   2391  O   GLN B 354     11.786  16.188  44.441  1.00 27.31           O
ATOM   2392  N   GLY B 355     13.496  17.303  45.431  1.00 24.17           N
ATOM   2393  CA  GLY B 355     13.551  16.367  46.542  1.00 26.73           C
ATOM   2394  C   GLY B 355     14.388  16.954  47.667  1.00 29.41           C
ATOM   2395  O   GLY B 355     14.773  18.123  47.626  1.00 24.83           O
ATOM   2396  N   VAL B 356     14.651  16.125  48.684  1.00 29.40           N
ATOM   2397  CA  VAL B 356     15.476  16.534  49.817  1.00 27.26           C
ATOM   2398  CB  VAL B 356     14.633  16.754  51.105  1.00 32.61           C
ATOM   2399  CG1 VAL B 356     15.549  17.148  52.284  1.00 32.35           C
ATOM   2400  CG2 VAL B 356     13.611  17.822  50.855  1.00 32.47           C
ATOM   2401  C   VAL B 356     16.446  15.389  50.059  1.00 21.33           C
ATOM   2402  O   VAL B 356     16.077  14.233  49.936  1.00 25.09           O
ATOM   2403  N   TYR B 357     17.690  15.724  50.382  1.00 29.52           N
ATOM   2404  CA  TYR B 357     18.705  14.706  50.643  1.00 30.43           C
ATOM   2405  CB  TYR B 357     19.852  14.784  49.631  1.00 35.80           C
ATOM   2406  CG  TYR B 357     20.948  13.782  49.918  1.00 33.13           C
ATOM   2407  CD1 TYR B 357     20.784  12.426  49.633  1.00 34.25           C
ATOM   2408  CE1 TYR B 357     21.789  11.496  49.933  1.00 38.44           C
ATOM   2409  CD2 TYR B 357     22.135  14.192  50.510  1.00 40.34           C
ATOM   2410  CE2 TYR B 357     23.143  13.274  50.816  1.00 39.74           C
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ATOM   2411  CZ   TYR B 357      22.964  11.935  50.524  1.00 39.72          C
ATOM   2412  OH   TYR B 357      23.971  11.048  50.819  1.00 49.57          O
ATOM   2413  C    TYR B 357      19.266  14.944  52.034  1.00 33.64          C
ATOM   2414  O    TYR B 357      19.528  16.085  52.420  1.00 32.19          O
ATOM   2415  N    ARG B 358      19.461  13.863  52.777  1.00 39.19          N
ATOM   2416  CA   ARG B 358      19.975  13.990  54.133  1.00 42.57          C
ATOM   2417  CB   ARG B 358      19.248  13.003  55.061  1.00 40.77          C
ATOM   2418  CG   ARG B 358      19.743  13.027  56.509  1.00 46.82          C
ATOM   2419  CD   ARG B 358      18.942  12.054  57.364  1.00 45.02          C
ATOM   2420  NE   ARG B 358      18.989  10.695  56.828  1.00 44.71          N
ATOM   2421  CZ   ARG B 358      18.075   9.765  57.089  1.00 45.22          C
ATOM   2422  NH1  ARG B 358      17.048  10.048  57.875  1.00 46.71          N
ATOM   2423  NH2  ARG B 358      18.184   8.548  56.564  1.00 47.43          N
ATOM   2424  C    ARG B 358      21.475  13.760  54.228  1.00 37.12          C
ATOM   2425  O    ARG B 358      21.957  12.680  53.901  1.00 38.27          O
ATOM   2426  N    MET B 359      22.198  14.798  54.643  1.00 48.39          N
ATOM   2427  CA   MET B 359      23.641  14.713  54.854  1.00 52.85          C
ATOM   2428  CB   MET B 359      24.368  15.892  54.211  1.00 56.92          C
ATOM   2429  CG   MET B 359      24.070  16.084  52.741  1.00 60.92          C
ATOM   2430  SD   MET B 359      25.113  17.339  51.987  1.00 69.39          S
ATOM   2431  CE   MET B 359      24.465  18.838  52.768  1.00 66.46          C
ATOM   2432  C    MET B 359      23.745  14.820  56.371  1.00 57.53          C
ATOM   2433  O    MET B 359      23.423  15.866  56.936  1.00 66.72          O
ATOM   2434  N    ARG B 360      24.163  13.741  57.024  1.00 61.83          N
ATOM   2435  CA   ARG B 360      24.269  13.706  58.488  1.00 63.23          C
ATOM   2436  CB   ARG B 360      25.166  12.537  58.925  1.00 63.83          C
ATOM   2437  CG   ARG B 360      24.590  11.170  58.552  1.00 65.58          C
ATOM   2438  CD   ARG B 360      23.197  11.000  59.158  1.00 65.50          C
ATOM   2439  NE   ARG B 360      22.294  10.220  58.310  1.00 64.72          N
ATOM   2440  CZ   ARG B 360      22.467   8.936  57.995  1.00 63.90          C
ATOM   2441  NH1  ARG B 360      23.523   8.261  58.451  1.00 62.73          N
ATOM   2442  NH2  ARG B 360      21.573   8.317  57.233  1.00 62.15          N
ATOM   2443  C    ARG B 360      24.765  15.008  59.099  1.00 61.92          C
ATOM   2444  O    ARG B 360      25.971  15.181  59.320  1.00 68.74          O
ATOM   2445  N    LYS B 361      23.811  15.905  59.374  1.00 58.30          N
ATOM   2446  CA   LYS B 361      24.045  17.233  59.948  1.00 55.64          C
ATOM   2447  CB   LYS B 361      25.338  17.844  59.389  1.00 60.30          C
ATOM   2448  CG   LYS B 361      25.334  18.061  57.877  1.00 60.80          C
ATOM   2449  CD   LYS B 361      26.738  18.379  57.338  1.00 63.13          C
ATOM   2450  CE   LYS B 361      27.334  19.641  57.964  1.00 63.56          C
ATOM   2451  NZ   LYS B 361      28.715  19.918  57.453  1.00 66.04          N
ATOM   2452  C    LYS B 361      22.857  18.139  59.589  1.00 60.03          C
ATOM   2453  O    LYS B 361      22.408  18.968  60.395  1.00 59.15          O
ATOM   2454  N    LYS B 362      22.353  17.971  58.365  1.00 53.10          N
ATOM   2455  CA   LYS B 362      21.225  18.756  57.878  1.00 55.57          C
ATOM   2456  CB   LYS B 362      21.661  20.202  57.665  1.00 57.57          C
ATOM   2457  CG   LYS B 362      22.780  20.355  56.656  1.00 54.04          C
ATOM   2458  CD   LYS B 362      23.226  21.799  56.608  1.00 58.13          C
ATOM   2459  CE   LYS B 362      24.111  22.049  55.408  1.00 60.20          C
ATOM   2460  NZ   LYS B 362      25.278  21.126  55.386  1.00 60.23          N
ATOM   2461  C    LYS B 362      20.659  18.192  56.571  1.00 48.43          C
ATOM   2462  O    LYS B 362      21.259  17.329  55.945  1.00 47.21          O
ATOM   2463  N    GLN B 363      19.490  18.675  56.168  1.00 51.49          N
ATOM   2464  CA   GLN B 363      18.877  18.200  54.935  1.00 49.86          C
ATOM   2465  CB   GLN B 363      17.463  17.662  55.190  1.00 56.81          C
ATOM   2466  CG   GLN B 363      17.400  16.534  56.212  1.00 54.91          C
ATOM   2467  CD   GLN B 363      16.007  15.927  56.325  1.00 55.16          C
ATOM   2468  OE1  GLN B 363      15.000  16.600  56.098  1.00 61.00          O
ATOM   2469  NE2  GLN B 363      15.947  14.658  56.692  1.00 58.13          N
ATOM   2470  C    GLN B 363      18.824  19.341  53.943  1.00 48.03          C
ATOM   2471  O    GLN B 363      18.369  20.435  54.261  1.00 50.07          O
ATOM   2472  N    ILE B 364      19.287  19.079  52.727  1.00 39.54          N
ATOM   2473  CA   ILE B 364      19.294  20.120  51.725  1.00 40.83          C
ATOM   2474  CB   ILE B 364      20.699  20.335  51.165  1.00 45.38          C
ATOM   2475  CG2  ILE B 364      21.653  20.714  52.290  1.00 41.39          C
ATOM   2476  CG1  ILE B 364      21.174  19.071  50.475  1.00 39.09          C
ATOM   2477  CD1  ILE B 364      22.299  19.333  49.517  1.00 48.16          C
ATOM   2478  C    ILE B 364      18.361  19.817  50.574  1.00 36.23          C
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ATOM	2479	O	ILE	B	364	18.086	18.656	50.268	1.00	30.72	O
ATOM	2480	N	ASP	B	365	17.875	20.870	49.934	1.00	35.72	N
ATOM	2481	CA	ASP	B	365	16.983	20.700	48.797	1.00	33.63	C
ATOM	2482	CB	ASP	B	365	16.300	22.025	48.483	1.00	37.07	C
ATOM	2483	CG	ASP	B	365	15.425	22.506	49.621	1.00	43.21	C
ATOM	2484	OD1	ASP	B	365	14.589	21.712	50.105	1.00	44.93	O
ATOM	2485	OD2	ASP	B	365	15.576	23.678	50.026	1.00	47.38	O
ATOM	2486	C	ASP	B	365	17.825	20.269	47.590	1.00	29.49	C
ATOM	2487	O	ASP	B	365	18.899	20.819	47.363	1.00	32.88	O
ATOM	2488	N	VAL	B	366	17.340	19.303	46.816	1.00	24.92	N
ATOM	2489	CA	VAL	B	366	18.080	18.847	45.653	1.00	25.63	C
ATOM	2490	CB	VAL	B	366	18.718	17.443	45.885	1.00	22.38	C
ATOM	2491	CG1	VAL	B	366	19.793	17.506	46.993	1.00	22.29	C
ATOM	2492	CG2	VAL	B	366	17.619	16.405	46.205	1.00	24.67	C
ATOM	2493	C	VAL	B	366	17.190	18.731	44.420	1.00	23.28	C
ATOM	2494	O	VAL	B	366	15.974	18.745	44.522	1.00	26.31	O
ATOM	2495	N	ALA	B	367	17.816	18.653	43.250	1.00	23.51	N
ATOM	2496	CA	ALA	B	367	17.091	18.439	42.010	1.00	26.78	C
ATOM	2497	CB	ALA	B	367	17.396	19.567	40.990	1.00	25.36	C
ATOM	2498	C	ALA	B	367	17.639	17.074	41.554	1.00	26.08	C
ATOM	2499	O	ALA	B	367	18.843	16.821	41.602	1.00	30.40	O
ATOM	2500	N	ILE	B	368	16.751	16.192	41.128	1.00	25.61	N
ATOM	2501	CA	ILE	B	368	17.124	14.839	40.735	1.00	25.37	C
ATOM	2502	CB	ILE	B	368	16.365	13.781	41.603	1.00	28.96	C
ATOM	2503	CG2	ILE	B	368	16.853	12.365	41.280	1.00	26.27	C
ATOM	2504	CG1	ILE	B	368	16.580	14.082	43.092	1.00	26.82	C
ATOM	2505	CD1	ILE	B	368	15.300	14.229	43.893	1.00	35.04	C
ATOM	2506	C	ILE	B	368	16.796	14.548	39.284	1.00	23.83	C
ATOM	2507	O	ILE	B	368	15.638	14.575	38.895	1.00	24.17	O
ATOM	2508	N	LYS	B	369	17.820	14.261	38.491	1.00	25.66	N
ATOM	2509	CA	LYS	B	369	17.593	13.923	37.089	1.00	26.48	C
ATOM	2510	CB	LYS	B	369	18.853	14.235	36.278	1.00	26.70	C
ATOM	2511	CG	LYS	B	369	18.727	13.997	34.804	1.00	32.20	C
ATOM	2512	CD	LYS	B	369	20.041	14.364	34.094	1.00	31.43	C
ATOM	2513	CE	LYS	B	369	20.013	13.896	32.654	1.00	37.28	C
ATOM	2514	NZ	LYS	B	369	21.184	14.385	31.848	1.00	31.40	N
ATOM	2515	C	LYS	B	369	17.250	12.429	37.070	1.00	30.56	C
ATOM	2516	O	LYS	B	369	18.079	11.572	37.414	1.00	29.63	O
ATOM	2517	N	VAL	B	370	16.016	12.112	36.703	1.00	28.76	N
ATOM	2518	CA	VAL	B	370	15.553	10.730	36.690	1.00	29.89	C
ATOM	2519	CB	VAL	B	370	14.192	10.594	37.410	1.00	32.92	C
ATOM	2520	CG1	VAL	B	370	13.824	9.133	37.553	1.00	38.36	C
ATOM	2521	CG2	VAL	B	370	14.235	11.289	38.775	1.00	31.30	C
ATOM	2522	C	VAL	B	370	15.391	10.222	35.265	1.00	33.31	C
ATOM	2523	O	VAL	B	370	14.623	10.779	34.484	1.00	33.69	O
ATOM	2524	N	LEU	B	371	16.110	9.166	34.921	1.00	32.83	N
ATOM	2525	CA	LEU	B	371	15.992	8.614	33.580	1.00	37.54	C
ATOM	2526	CB	LEU	B	371	17.164	7.676	33.288	1.00	39.83	C
ATOM	2527	CG	LEU	B	371	18.543	8.328	33.234	1.00	40.84	C
ATOM	2528	CD1	LEU	B	371	19.589	7.261	32.948	1.00	41.39	C
ATOM	2529	CD2	LEU	B	371	18.555	9.402	32.166	1.00	39.76	C
ATOM	2530	C	LEU	B	371	14.675	7.853	33.449	1.00	43.14	C
ATOM	2531	O	LEU	B	371	14.307	7.075	34.339	1.00	39.21	O
ATOM	2532	N	LYS	B	372	13.978	8.075	32.337	1.00	41.93	N
ATOM	2533	CA	LYS	B	372	12.699	7.420	32.080	1.00	47.49	C
ATOM	2534	CB	LYS	B	372	12.114	7.917	30.756	1.00	49.29	C
ATOM	2535	CG	LYS	B	372	13.009	7.677	29.541	1.00	52.95	C
ATOM	2536	CD	LYS	B	372	12.390	8.257	28.275	1.00	54.13	C
ATOM	2537	CE	LYS	B	372	13.254	7.957	27.057	1.00	57.77	C
ATOM	2538	NZ	LYS	B	372	12.655	8.487	25.796	1.00	61.32	N
ATOM	2539	C	LYS	B	372	12.851	5.900	32.052	1.00	52.52	C
ATOM	2540	O	LYS	B	372	13.951	5.378	31.877	1.00	47.39	O
ATOM	2541	N	GLN	B	373	11.740	5.193	32.238	1.00	59.30	N
ATOM	2542	CA	GLN	B	373	11.755	3.733	32.231	1.00	59.74	C
ATOM	2543	CB	GLN	B	373	10.418	3.197	32.762	1.00	64.02	C
ATOM	2544	CG	GLN	B	373	10.377	1.685	32.981	1.00	66.26	C
ATOM	2545	CD	GLN	B	373	11.342	1.215	34.063	1.00	70.74	C
ATOM	2546	OE1	GLN	B	373	12.562	1.337	33.924	1.00	69.05	O

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ATOM	2547	NE2	GLN	B	373	10.795	0.672	35.147	1.00	69.07	N
ATOM	2548	C	GLN	B	373	12.005	3.213	30.811	1.00	61.28	C
ATOM	2549	O	GLN	B	373	11.441	3.728	29.840	1.00	59.36	O
ATOM	2550	N	GLY	B	374	12.863	2.203	30.692	1.00	60.31	N
ATOM	2551	CA	GLY	B	374	13.160	1.645	29.385	1.00	62.87	C
ATOM	2552	C	GLY	B	374	14.425	2.207	28.763	1.00	64.46	C
ATOM	2553	O	GLY	B	374	14.792	1.838	27.643	1.00	64.42	O
ATOM	2554	N	THR	B	375	15.091	3.101	29.490	1.00	62.61	N
ATOM	2555	CA	THR	B	375	16.326	3.722	29.019	1.00	62.15	C
ATOM	2556	CB	THR	B	375	16.913	4.678	30.089	1.00	61.37	C
ATOM	2557	OG1	THR	B	375	16.039	5.799	30.268	1.00	57.85	O
ATOM	2558	CG2	THR	B	375	18.288	5.175	29.671	1.00	61.31	C
ATOM	2559	C	THR	B	375	17.374	2.666	28.673	1.00	60.79	C
ATOM	2560	O	THR	B	375	17.728	1.835	29.507	1.00	61.50	O
ATOM	2561	N	GLU	B	376	17.867	2.708	27.440	1.00	61.17	N
ATOM	2562	CA	GLU	B	376	18.874	1.753	26.990	1.00	63.67	C
ATOM	2563	CB	GLU	B	376	19.139	1.933	25.496	1.00	65.15	C
ATOM	2564	CG	GLU	B	376	20.120	0.923	24.917	1.00	71.18	C
ATOM	2565	CD	GLU	B	376	20.089	0.883	23.398	1.00	73.78	C
ATOM	2566	OE1	GLU	B	376	20.380	1.923	22.758	1.00	72.53	O
ATOM	2567	OE2	GLU	B	376	19.769	-0.193	22.843	1.00	73.05	O
ATOM	2568	C	GLU	B	376	20.169	1.943	27.771	1.00	65.33	C
ATOM	2569	O	GLU	B	376	20.462	3.046	28.237	1.00	61.91	O
ATOM	2570	N	LYS	B	377	20.940	0.868	27.910	1.00	59.58	N
ATOM	2571	CA	LYS	B	377	22.196	0.927	28.644	1.00	61.29	C
ATOM	2572	CB	LYS	B	377	22.896	-0.432	28.608	1.00	65.21	C
ATOM	2573	CG	LYS	B	377	24.222	-0.454	29.356	1.00	65.59	C
ATOM	2574	CD	LYS	B	377	24.611	-1.872	29.736	1.00	71.26	C
ATOM	2575	CE	LYS	B	377	25.867	-1.896	30.599	1.00	70.47	C
ATOM	2576	NZ	LYS	B	377	26.267	-3.292	30.962	1.00	72.53	N
ATOM	2577	C	LYS	B	377	23.131	1.993	28.095	1.00	59.78	C
ATOM	2578	O	LYS	B	377	23.999	2.497	28.808	1.00	56.95	O
ATOM	2579	N	ALA	B	378	22.952	2.329	26.823	1.00	61.07	N
ATOM	2580	CA	ALA	B	378	23.777	3.337	26.168	1.00	59.33	C
ATOM	2581	CB	ALA	B	378	23.399	3.435	24.695	1.00	59.59	C
ATOM	2582	C	ALA	B	378	23.624	4.703	26.836	1.00	57.38	C
ATOM	2583	O	ALA	B	378	24.612	5.376	27.138	1.00	56.25	O
ATOM	2584	N	ASP	B	379	22.380	5.098	27.075	1.00	57.35	N
ATOM	2585	CA	ASP	B	379	22.094	6.388	27.691	1.00	59.15	C
ATOM	2586	CB	ASP	B	379	20.650	6.788	27.416	1.00	61.51	C
ATOM	2587	CG	ASP	B	379	20.151	6.255	26.088	1.00	68.59	C
ATOM	2588	OD1	ASP	B	379	20.739	6.601	25.035	1.00	70.20	O
ATOM	2589	OD2	ASP	B	379	19.168	5.479	26.098	1.00	70.89	O
ATOM	2590	C	ASP	B	379	22.341	6.358	29.197	1.00	56.77	C
ATOM	2591	O	ASP	B	379	22.596	7.392	29.811	1.00	53.33	O
ATOM	2592	N	THR	B	380	22.258	5.170	29.790	1.00	52.16	N
ATOM	2593	CA	THR	B	380	22.513	5.019	31.215	1.00	53.38	C
ATOM	2594	CB	THR	B	380	22.187	3.590	31.684	1.00	53.55	C
ATOM	2595	OG1	THR	B	380	20.768	3.391	31.641	1.00	54.68	O
ATOM	2596	CG2	THR	B	380	22.683	3.371	33.096	1.00	58.07	C
ATOM	2597	C	THR	B	380	23.998	5.295	31.432	1.00	52.60	C
ATOM	2598	O	THR	B	380	24.390	5.980	32.374	1.00	48.13	O
ATOM	2599	N	GLU	B	381	24.819	4.752	30.540	1.00	46.95	N
ATOM	2600	CA	GLU	B	381	26.260	4.937	30.617	1.00	49.11	C
ATOM	2601	CB	GLU	B	381	26.955	4.060	29.573	1.00	54.95	C
ATOM	2602	CG	GLU	B	381	28.020	3.129	30.134	1.00	58.45	C
ATOM	2603	CD	GLU	B	381	27.442	1.927	30.862	1.00	65.92	C
ATOM	2604	OE1	GLU	B	381	26.790	2.114	31.913	1.00	66.10	O
ATOM	2605	OE2	GLU	B	381	27.644	0.788	30.377	1.00	67.00	O
ATOM	2606	C	GLU	B	381	26.559	6.412	30.343	1.00	45.43	C
ATOM	2607	O	GLU	B	381	27.518	6.974	30.864	1.00	40.91	O
ATOM	2608	N	GLU	B	382	25.716	7.029	29.525	1.00	43.34	N
ATOM	2609	CA	GLU	B	382	25.871	8.435	29.164	1.00	45.73	C
ATOM	2610	CB	GLU	B	382	24.842	8.795	28.099	1.00	50.57	C
ATOM	2611	CG	GLU	B	382	24.988	10.184	27.524	1.00	55.43	C
ATOM	2612	CD	GLU	B	382	24.064	10.410	26.336	1.00	60.92	C
ATOM	2613	OE1	GLU	B	382	22.825	10.449	26.528	1.00	67.80	C
ATOM	2614	OE2	GLU	B	382	24.580	10.536	25.203	1.00	65.61	O

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ATOM   2615  C    GLU B 382    25.696    9.331   30.394  1.00 42.57       C
ATOM   2616  O    GLU B 382    26.444   10.294   30.587  1.00 36.66       O
ATOM   2617  N    MET B 383    24.700    9.017   31.217  1.00 36.27       N
ATOM   2618  CA   MET B 383    24.482    9.806   32.417  1.00 36.21       C
ATOM   2619  CB   MET B 383    23.116    9.489   33.051  1.00 37.94       C
ATOM   2620  CG   MET B 383    22.686   10.580   34.040  1.00 45.05       S
ATOM   2621  SD   MET B 383    21.039   10.380   34.734  1.00 49.17       C
ATOM   2622  CE   MET B 383    21.377    9.057   35.776  1.00 31.72       O
ATOM   2623  C    MET B 383    25.602    9.543   33.420  1.00 32.29       N
ATOM   2624  O    MET B 383    25.912   10.389   34.245  1.00 27.76       C
ATOM   2625  N    MET B 384    26.212    8.361   33.362  1.00 32.45       C
ATOM   2626  CA   MET B 384    27.310    8.076   34.276  1.00 34.42       S
ATOM   2627  CB   MET B 384    27.664    6.588   34.262  1.00 38.83       C
ATOM   2628  CG   MET B 384    26.634    5.702   34.943  1.00 41.15       C
ATOM   2629  SD   MET B 384    26.295    6.179   36.672  1.00 47.37       O
ATOM   2630  CE   MET B 384    27.936    6.041   37.407  1.00 46.98       N
ATOM   2631  C    MET B 384    28.529    8.911   33.896  1.00 31.48       C
ATOM   2632  O    MET B 384    29.284    9.352   34.762  1.00 31.65       C
ATOM   2633  N    ARG B 385    28.727    9.133   32.603  1.00 34.67       C
ATOM   2634  CA   ARG B 385    29.848    9.962   32.172  1.00 36.33       N
ATOM   2635  CB   ARG B 385    30.011    9.926   30.652  1.00 37.82       C
ATOM   2636  CG   ARG B 385    30.687    8.667   30.129  1.00 45.45       N
ATOM   2637  CD   ARG B 385    31.105    8.837   28.665  1.00 46.60       N
ATOM   2638  NE   ARG B 385    29.969    8.752   27.756  1.00 45.85       C
ATOM   2639  CZ   ARG B 385    29.377    7.610   27.417  1.00 47.08       O
ATOM   2640  NH1  ARG B 385    29.823    6.459   27.913  1.00 48.61       N
ATOM   2641  NH2  ARG B 385    28.342    7.612   26.592  1.00 46.74       C
ATOM   2642  C    ARG B 385    29.596   11.391   32.636  1.00 29.96       C
ATOM   2643  O    ARG B 385    30.520   12.098   33.021  1.00 33.63       C
ATOM   2644  N    GLU B 386    28.330   11.799   32.612  1.00 30.00       O
ATOM   2645  CA   GLU B 386    27.948   13.141   33.051  1.00 29.80       C
ATOM   2646  CB   GLU B 386    26.447   13.368   32.790  1.00 27.12       O
ATOM   2647  CG   GLU B 386    25.882   14.720   33.233  1.00 32.18       C
ATOM   2648  CD   GLU B 386    24.372   14.825   32.961  1.00 35.05       N
ATOM   2649  OE1  GLU B 386    23.801   13.830   32.475  1.00 34.50       C
ATOM   2650  OE2  GLU B 386    23.756   15.890   33.251  1.00 35.81       C
ATOM   2651  C    GLU B 386    28.259   13.298   34.540  1.00 28.79       C
ATOM   2652  O    GLU B 386    28.752   14.350   34.986  1.00 26.92       O
ATOM   2653  N    ALA B 387    27.967   12.253   35.305  1.00 30.29       N
ATOM   2654  CA   ALA B 387    28.223   12.295   36.736  1.00 33.27       C
ATOM   2655  CB   ALA B 387    27.644   11.044   37.421  1.00 30.95       C
ATOM   2656  C    ALA B 387    29.744   12.398   36.962  1.00 26.41       C
ATOM   2657  O    ALA B 387    30.191   13.182   37.774  1.00 35.19       O
ATOM   2658  N    GLN B 388    30.518   11.614   36.219  1.00 32.50       N
ATOM   2659  CA   GLN B 388    31.984   11.654   36.367  1.00 37.92       C
ATOM   2660  CB   GLN B 388    32.647   10.664   35.387  1.00 38.99       C
ATOM   2661  CG   GLN B 388    32.269    9.211   35.625  1.00 47.85       C
ATOM   2662  CD   GLN B 388    32.810    8.279   34.546  1.00 56.30       C
ATOM   2663  OE1  GLN B 388    34.016    8.248   34.281  1.00 56.71       O
ATOM   2664  NE2  GLN B 388    31.914    7.514   33.915  1.00 53.14       N
ATOM   2665  C    GLN B 388    32.546   13.060   36.134  1.00 35.03       C
ATOM   2666  O    GLN B 388    33.442   13.501   36.841  1.00 32.27       O
ATOM   2667  N    ILE B 389    32.015   13.767   35.135  1.00 30.85       N
ATOM   2668  CA   ILE B 389    32.463   15.130   34.840  1.00 25.41       C
ATOM   2669  CB   ILE B 389    31.853   15.645   33.499  1.00 32.74       C
ATOM   2670  CG2  ILE B 389    32.051   17.159   33.363  1.00 31.69       C
ATOM   2671  CG1  ILE B 389    32.505   14.906   32.328  1.00 38.87       C
ATOM   2672  CD1  ILE B 389    31.893   15.236   30.982  1.00 36.36       C
ATOM   2673  C    ILE B 389    32.072   16.074   35.949  1.00 26.93       C
ATOM   2674  O    ILE B 389    32.872   16.886   36.411  1.00 30.11       O
ATOM   2675  N    MET B 390    30.832   15.978   36.403  1.00 26.48       N
ATOM   2676  CA   MET B 390    30.398   16.857   37.459  1.00 24.57       C
ATOM   2677  CB   MET B 390    28.906   16.695   37.735  1.00 24.91       C
ATOM   2678  CG   MET B 390    28.002   17.248   36.638  1.00 26.56       C
ATOM   2679  SD   MET B 390    26.239   17.032   37.117  1.00 30.07       S
ATOM   2680  CE   MET B 390    26.009   18.455   38.144  1.00 31.13       C
ATOM   2681  C    MET B 390    31.186   16.563   38.738  1.00 30.37       C
ATOM   2682  O    MET B 390    31.506   17.484   39.487  1.00 29.10       O
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ATOM	2683	N	HIS	B	391	31.497	15.286	38.956	1.00	31.09	N
ATOM	2684	CA	HIS	B	391	32.243	14.890	40.160	1.00	37.62	C
ATOM	2685	CB	HIS	B	391	32.285	13.358	40.270	1.00	42.66	C
ATOM	2686	CG	HIS	B	391	32.831	12.854	41.573	1.00	50.59	C
ATOM	2687	CD2	HIS	B	391	32.206	12.397	42.686	1.00	51.17	N
ATOM	2688	ND1	HIS	B	391	34.182	12.815	41.850	1.00	56.54	C
ATOM	2689	CE1	HIS	B	391	34.366	12.356	43.076	1.00	56.46	N
ATOM	2690	NE2	HIS	B	391	33.183	12.094	43.605	1.00	57.11	C
ATOM	2691	C	HIS	B	391	33.661	15.454	40.155	1.00	43.32	O
ATOM	2692	O	HIS	B	391	34.338	15.452	41.182	1.00	47.18	N
ATOM	2693	N	GLN	B	392	34.111	15.941	38.999	1.00	39.89	C
ATOM	2694	CA	GLN	B	392	35.449	16.516	38.886	1.00	40.61	C
ATOM	2695	CB	GLN	B	392	36.094	16.110	37.557	1.00	42.86	C
ATOM	2696	CG	GLN	B	392	36.181	14.610	37.364	1.00	47.64	O
ATOM	2697	CD	GLN	B	392	36.948	14.219	36.129	1.00	50.73	C
ATOM	2698	OE1	GLN	B	392	38.161	14.408	36.058	1.00	60.38	O
ATOM	2699	NE2	GLN	B	392	36.250	13.664	35.145	1.00	48.83	N
ATOM	2700	C	GLN	B	392	35.415	18.031	38.987	1.00	47.76	C
ATOM	2701	O	GLN	B	392	36.444	18.689	38.850	1.00	46.42	C
ATOM	2702	N	LEU	B	393	34.233	18.586	39.240	1.00	45.72	C
ATOM	2703	CA	LEU	B	393	34.069	20.034	39.342	1.00	45.69	C
ATOM	2704	CB	LEU	B	393	32.909	20.491	38.454	1.00	44.69	C
ATOM	2705	CG	LEU	B	393	32.913	20.011	37.000	1.00	46.90	C
ATOM	2706	CD1	LEU	B	393	31.656	20.508	36.312	1.00	44.79	C
ATOM	2707	CD2	LEU	B	393	34.153	20.507	36.281	1.00	37.05	O
ATOM	2708	C	LEU	B	393	33.826	20.515	40.770	1.00	45.06	N
ATOM	2709	O	LEU	B	393	33.044	19.928	41.523	1.00	49.45	C
ATOM	2710	N	ASP	B	394	34.481	21.603	41.151	1.00	43.03	C
ATOM	2711	CA	ASP	B	394	34.315	22.133	42.495	1.00	36.00	C
ATOM	2712	CB	ASP	B	394	35.432	21.600	43.403	1.00	47.00	O
ATOM	2713	CG	ASP	B	394	35.292	22.063	44.844	1.00	52.54	C
ATOM	2714	OD1	ASP	B	394	36.167	21.705	45.668	1.00	55.59	O
ATOM	2715	OD2	ASP	B	394	34.315	22.774	45.160	1.00	47.08	O
ATOM	2716	C	ASP	B	394	34.381	23.640	42.427	1.00	40.50	C
ATOM	2717	O	ASP	B	394	35.434	24.247	42.671	1.00	38.62	O
ATOM	2718	N	ASN	B	395	33.251	24.254	42.105	1.00	35.95	N
ATOM	2719	CA	ASN	B	395	33.216	25.699	41.987	1.00	31.17	C
ATOM	2720	CB	ASN	B	395	33.463	26.092	40.518	1.00	25.15	C
ATOM	2721	CG	ASN	B	395	33.595	27.578	40.328	1.00	36.48	C
ATOM	2722	OD1	ASN	B	395	34.673	28.158	40.523	1.00	37.23	O
ATOM	2723	ND2	ASN	B	395	32.497	28.217	39.950	1.00	25.99	N
ATOM	2724	C	ASN	B	395	31.851	26.171	42.458	1.00	30.67	C
ATOM	2725	O	ASN	B	395	30.821	25.528	42.197	1.00	28.65	O
ATOM	2726	N	PRO	B	396	31.822	27.315	43.147	1.00	27.83	N
ATOM	2727	CD	PRO	B	396	32.966	28.068	43.680	1.00	37.81	C
ATOM	2728	CA	PRO	B	396	30.570	27.867	43.655	1.00	26.99	C
ATOM	2729	CB	PRO	B	396	31.036	29.053	44.483	1.00	35.20	C
ATOM	2730	CG	PRO	B	396	32.414	28.620	44.946	1.00	41.91	C
ATOM	2731	C	PRO	B	396	29.568	28.291	42.579	1.00	29.09	C
ATOM	2732	O	PRO	B	396	28.402	28.428	42.865	1.00	26.93	O
ATOM	2733	N	TYR	B	397	30.043	28.485	41.343	1.00	24.67	N
ATOM	2734	CA	TYR	B	397	29.145	28.956	40.263	1.00	24.00	C
ATOM	2735	CB	TYR	B	397	29.827	30.136	39.545	1.00	23.32	C
ATOM	2736	CG	TYR	B	397	30.228	31.229	40.524	1.00	26.27	C
ATOM	2737	CD1	TYR	B	397	31.568	31.425	40.881	1.00	26.92	C
ATOM	2738	CE1	TYR	B	397	31.929	32.379	41.823	1.00	31.33	C
ATOM	2739	CD2	TYR	B	397	29.266	32.024	41.136	1.00	25.87	C
ATOM	2740	CE2	TYR	B	397	29.620	32.987	42.085	1.00	33.47	C
ATOM	2741	CZ	TYR	B	397	30.950	33.155	42.426	1.00	34.44	C
ATOM	2742	OH	TYR	B	397	31.263	34.067	43.411	1.00	37.25	O
ATOM	2743	C	TYR	B	397	28.694	27.893	39.294	1.00	23.67	C
ATOM	2744	O	TYR	B	397	28.286	28.165	38.135	1.00	24.69	O
ATOM	2745	N	ILE	B	398	28.755	26.659	39.752	1.00	21.85	N
ATOM	2746	CA	ILE	B	398	28.336	25.519	38.991	1.00	26.71	C
ATOM	2747	CB	ILE	B	398	29.567	24.716	38.567	1.00	34.69	C
ATOM	2748	CG2	ILE	B	398	29.165	23.359	38.073	1.00	36.71	C
ATOM	2749	CG1	ILE	B	398	30.332	25.501	37.498	1.00	28.39	C
ATOM	2750	CD1	ILE	B	398	31.737	25.021	37.232	1.00	39.03	C

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                                        atomic coordinates.txt
ATOM   2751  C   ILE B 398      27.421  24.691  39.906  1.00 34.83           C
ATOM   2752  O   ILE B 398      27.640  24.636  41.120  1.00 31.60           O
ATOM   2753  N   VAL B 399      26.378  24.103  39.333  1.00 26.19           N
ATOM   2754  CA  VAL B 399      25.458  23.243  40.086  1.00 29.92           C
ATOM   2755  CB  VAL B 399      24.272  22.781  39.232  1.00 30.42           C
ATOM   2756  CG1 VAL B 399      23.498  21.627  39.946  1.00 29.50           C
ATOM   2757  CG2 VAL B 399      23.360  23.960  38.970  1.00 31.26           C
ATOM   2758  C   VAL B 399      26.265  22.016  40.464  1.00 34.54           C
ATOM   2759  O   VAL B 399      26.697  21.269  39.597  1.00 35.65           O
ATOM   2760  N   ARG B 400      26.430  21.805  41.763  1.00 27.76           N
ATOM   2761  CA  ARG B 400      27.227  20.683  42.244  1.00 32.53           C
ATOM   2762  CB  ARG B 400      27.744  20.994  43.658  1.00 38.09           C
ATOM   2763  CG  ARG B 400      28.606  22.262  43.787  1.00 46.29           C
ATOM   2764  CD  ARG B 400      28.970  22.541  45.262  1.00 46.35           C
ATOM   2765  NE  ARG B 400      29.833  23.711  45.437  1.00 52.96           N
ATOM   2766  CZ  ARG B 400      31.116  23.743  45.092  1.00 55.68           C
ATOM   2767  NH1 ARG B 400      31.675  22.666  44.557  1.00 51.73           N
ATOM   2768  NH2 ARG B 400      31.841  24.847  45.278  1.00 52.56           N
ATOM   2769  C   ARG B 400      26.513  19.345  42.256  1.00 27.44           C
ATOM   2770  O   ARG B 400      25.313  19.254  42.507  1.00 28.50           O
ATOM   2771  N   LEU B 401      27.259  18.280  42.006  1.00 27.68           N
ATOM   2772  CA  LEU B 401      26.695  16.948  42.018  1.00 24.03           C
ATOM   2773  CB  LEU B 401      27.514  16.006  41.156  1.00 32.24           C
ATOM   2774  CG  LEU B 401      27.086  14.540  41.184  1.00 29.66           C
ATOM   2775  CD1 LEU B 401      25.713  14.354  40.554  1.00 35.88           C
ATOM   2776  CD2 LEU B 401      28.132  13.737  40.425  1.00 39.27           C
ATOM   2777  C   LEU B 401      26.745  16.426  43.456  1.00 35.79           C
ATOM   2778  O   LEU B 401      27.796  16.487  44.103  1.00 29.49           O
ATOM   2779  N   ILE B 402      25.611  15.945  43.957  1.00 27.95           N
ATOM   2780  CA  ILE B 402      25.581  15.368  45.299  1.00 29.27           C
ATOM   2781  CB  ILE B 402      24.154  15.383  45.922  1.00 31.13           C
ATOM   2782  CG2 ILE B 402      24.188  14.716  47.305  1.00 33.30           C
ATOM   2783  CG1 ILE B 402      23.650  16.830  46.065  1.00 26.94           C
ATOM   2784  CD1 ILE B 402      24.616  17.763  46.743  1.00 31.79           C
ATOM   2785  C   ILE B 402      26.053  13.921  45.119  1.00 32.38           C
ATOM   2786  O   ILE B 402      26.962  13.448  45.812  1.00 31.53           O
ATOM   2787  N   GLY B 403      25.469  13.226  44.157  1.00 27.83           N
ATOM   2788  CA  GLY B 403      25.870  11.853  43.900  1.00 29.46           C
ATOM   2789  C   GLY B 403      24.897  11.150  42.994  1.00 29.35           C
ATOM   2790  O   GLY B 403      23.934  11.757  42.537  1.00 30.33           O
ATOM   2791  N   VAL B 404      25.145   9.878  42.717  1.00 26.15           N
ATOM   2792  CA  VAL B 404      24.281   9.084  41.865  1.00 28.12           C
ATOM   2793  CB  VAL B 404      25.106   8.273  40.844  1.00 36.04           C
ATOM   2794  CG1 VAL B 404      24.186   7.397  39.982  1.00 40.40           C
ATOM   2795  CG2 VAL B 404      25.911   9.211  39.982  1.00 35.87           C
ATOM   2796  C   VAL B 404      23.519   8.114  42.755  1.00 32.26           C
ATOM   2797  O   VAL B 404      24.052   7.647  43.744  1.00 31.47           O
ATOM   2798  N   CYS B 405      22.277   7.815  42.392  1.00 30.13           N
ATOM   2799  CA  CYS B 405      21.471   6.879  43.177  1.00 35.84           C
ATOM   2800  CB  CYS B 405      20.408   7.635  43.976  1.00 39.61           C
ATOM   2801  SG  CYS B 405      19.571   6.617  45.215  1.00 43.65           S
ATOM   2802  C   CYS B 405      20.815   5.849  42.258  1.00 41.06           C
ATOM   2803  O   CYS B 405      20.101   6.200  41.320  1.00 38.70           O
ATOM   2804  N   GLN B 406      21.086   4.577  42.510  1.00 41.04           N
ATOM   2805  CA  GLN B 406      20.529   3.511  41.687  1.00 49.92           C
ATOM   2806  CB  GLN B 406      21.639   2.549  41.250  1.00 53.55           C
ATOM   2807  CG  GLN B 406      21.165   1.355  40.413  1.00 59.57           C
ATOM   2808  CD  GLN B 406      20.378   1.756  39.169  1.00 56.22           C
ATOM   2809  OE1 GLN B 406      19.205   2.123  39.246  1.00 59.42           O
ATOM   2810  NE2 GLN B 406      21.028   1.687  38.016  1.00 59.35           N
ATOM   2811  C   GLN B 406      19.450   2.750  42.446  1.00 53.55           C
ATOM   2812  O   GLN B 406      19.746   1.894  43.273  1.00 56.70           O
ATOM   2813  N   ALA B 407      18.197   3.080  42.163  1.00 56.23           N
ATOM   2814  CA  ALA B 407      17.069   2.418  42.808  1.00 60.79           C
ATOM   2815  CB  ALA B 407      16.432   3.359  43.829  1.00 60.88           C
ATOM   2816  C   ALA B 407      16.052   2.012  41.742  1.00 58.91           C
ATOM   2817  O   ALA B 407      16.364   1.212  40.856  1.00 57.00           O
ATOM   2818  N   GLU B 408      14.846   2.568  41.821  1.00 55.11           N
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ATOM   2819  CA   GLU B 408       13.806    2.260   40.849  1.00 57.75      C
ATOM   2820  CB   GLU B 408       12.535    3.065   41.147  1.00 61.87      C
ATOM   2821  CG   GLU B 408       12.759    4.562   41.299  1.00 61.03      C
ATOM   2822  CD   GLU B 408       12.938    4.998   42.748  1.00 61.45      C
ATOM   2823  OE1  GLU B 408       13.788    4.422   43.464  1.00 62.30      O
ATOM   2824  OE2  GLU B 408       12.228    5.933   43.169  1.00 57.96      O
ATOM   2825  C    GLU B 408       14.320    2.590   39.452  1.00 58.74      C
ATOM   2826  O    GLU B 408       13.770    2.139   38.444  1.00 61.01      O
ATOM   2827  N    ALA B 409       15.383    3.387   39.408  1.00 58.64      N
ATOM   2828  CA   ALA B 409       16.017    3.788   38.159  1.00 53.23      C
ATOM   2829  CB   ALA B 409       15.054    4.621   37.327  1.00 57.75      C
ATOM   2830  C    ALA B 409       17.262    4.595   38.518  1.00 48.64      C
ATOM   2831  O    ALA B 409       17.451    4.957   39.682  1.00 41.77      O
ATOM   2832  N    LEU B 410       18.113    4.859   37.527  1.00 46.67      N
ATOM   2833  CA   LEU B 410       19.348    5.606   37.757  1.00 41.56      C
ATOM   2834  CB   LEU B 410       20.326    5.370   36.607  1.00 41.30      C
ATOM   2835  CG   LEU B 410       21.745    5.849   36.893  1.00 39.49      C
ATOM   2836  CD1  LEU B 410       22.282    5.132   38.127  1.00 40.07      C
ATOM   2837  CD2  LEU B 410       22.628    5.590   35.680  1.00 44.22      C
ATOM   2838  C    LEU B 410       19.024    7.087   37.877  1.00 36.27      C
ATOM   2839  O    LEU B 410       18.291    7.631   37.068  1.00 32.58      O
ATOM   2840  N    MET B 411       19.579    7.740   38.888  1.00 31.99      N
ATOM   2841  CA   MET B 411       19.277    9.144   39.105  1.00 28.85      C
ATOM   2842  CB   MET B 411       18.272    9.282   40.261  1.00 27.82      C
ATOM   2843  CG   MET B 411       16.998    8.467   40.120  1.00 38.03      C
ATOM   2844  SD   MET B 411       15.902    8.655   41.550  1.00 39.66      S
ATOM   2845  CE   MET B 411       16.875    7.893   42.769  1.00 39.08      C
ATOM   2846  C    MET B 411       20.518    9.931   39.454  1.00 34.64      C
ATOM   2847  O    MET B 411       21.415    9.412   40.110  1.00 32.86      O
ATOM   2848  N    LEU B 412       20.576   11.182   39.012  1.00 27.07      N
ATOM   2849  CA   LEU B 412       21.686   12.070   39.353  1.00 24.70      C
ATOM   2850  CB   LEU B 412       22.213   12.819   38.122  1.00 31.40      C
ATOM   2851  CG   LEU B 412       23.072   12.039   37.146  1.00 42.38      C
ATOM   2852  CD1  LEU B 412       23.695   13.008   36.127  1.00 40.09      C
ATOM   2853  CD2  LEU B 412       24.156   11.325   37.940  1.00 44.83      C
ATOM   2854  C    LEU B 412       21.108   13.086   40.316  1.00 32.72      C
ATOM   2855  O    LEU B 412       20.203   13.829   39.930  1.00 25.93      O
ATOM   2856  N    VAL B 413       21.632   13.118   41.552  1.00 25.13      N
ATOM   2857  CA   VAL B 413       21.179   14.048   42.591  1.00 22.67      C
ATOM   2858  CB   VAL B 413       21.169   13.374   43.997  1.00 27.42      C
ATOM   2859  CG1  VAL B 413       20.591   14.333   45.040  1.00 22.22      C
ATOM   2860  CG2  VAL B 413       20.369   12.079   43.932  1.00 27.93      C
ATOM   2861  C    VAL B 413       22.099   15.245   42.627  1.00 26.70      C
ATOM   2862  O    VAL B 413       23.317   15.115   42.869  1.00 28.13      O
ATOM   2863  N    MET B 414       21.503   16.417   42.414  1.00 23.91      N
ATOM   2864  CA   MET B 414       22.232   17.672   42.353  1.00 23.05      C
ATOM   2865  CB   MET B 414       22.146   18.241   40.913  1.00 26.27      C
ATOM   2866  CG   MET B 414       22.782   17.373   39.850  1.00 31.80      C
ATOM   2867  SD   MET B 414       22.187   17.909   38.179  1.00 31.87      S
ATOM   2868  CE   MET B 414       20.682   16.914   38.038  1.00 34.99      C
ATOM   2869  C    MET B 414       21.683   18.729   43.269  1.00 24.82      C
ATOM   2870  O    MET B 414       20.536   18.646   43.732  1.00 26.89      O
ATOM   2871  N    GLU B 415       22.475   19.767   43.508  1.00 22.82      N
ATOM   2872  CA   GLU B 415       22.008   20.867   44.330  1.00 25.46      C
ATOM   2873  CB   GLU B 415       23.089   21.939   44.500  1.00 38.09      C
ATOM   2874  CG   GLU B 415       24.381   21.466   45.121  1.00 41.76      C
ATOM   2875  CD   GLU B 415       25.406   22.600   45.191  1.00 56.15      C
ATOM   2876  OE1  GLU B 415       25.611   23.293   44.153  1.00 43.26      O
ATOM   2877  OE2  GLU B 415       26.000   22.796   46.279  1.00 53.48      O
ATOM   2878  C    GLU B 415       20.848   21.511   43.581  1.00 28.34      C
ATOM   2879  O    GLU B 415       20.819   21.496   42.347  1.00 27.84      O
ATOM   2880  N    MET B 416       19.903   22.079   44.327  1.00 28.24      N
ATOM   2881  CA   MET B 416       18.776   22.739   43.701  1.00 27.37      C
ATOM   2882  CB   MET B 416       17.482   22.444   44.452  1.00 31.26      C
ATOM   2883  CG   MET B 416       16.245   22.889   43.658  1.00 33.79      C
ATOM   2884  SD   MET B 416       14.717   22.640   44.566  1.00 40.24      S
ATOM   2885  CE   MET B 416       13.622   23.863   43.732  1.00 41.28      C
ATOM   2886  C    MET B 416       18.989   24.247   43.709  1.00 32.53      C
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ATOM	2887	O	MET	B	416	19.462	24.797	44.695	1.00	29.31	O
ATOM	2888	N	ALA	B	417	18.639	24.900	42.603	1.00	29.63	N
ATOM	2889	CA	ALA	B	417	18.724	26.362	42.497	1.00	32.11	C
ATOM	2890	CB	ALA	B	417	19.676	26.775	41.365	1.00	31.26	C
ATOM	2891	C	ALA	B	417	17.282	26.779	42.186	1.00	32.20	C
ATOM	2892	O	ALA	B	417	16.903	26.933	41.017	1.00	31.90	O
ATOM	2893	N	GLY	B	418	16.500	26.924	43.259	1.00	34.38	N
ATOM	2894	CA	GLY	B	418	15.081	27.243	43.183	1.00	36.34	C
ATOM	2895	C	GLY	B	418	14.630	28.461	42.398	1.00	34.85	C
ATOM	2896	O	GLY	B	418	13.447	28.598	42.082	1.00	34.44	O
ATOM	2897	N	GLY	B	419	15.563	29.359	42.105	1.00	28.57	N
ATOM	2898	CA	GLY	B	419	15.208	30.537	41.339	1.00	30.78	C
ATOM	2899	C	GLY	B	419	14.891	30.180	39.897	1.00	33.81	C
ATOM	2900	O	GLY	B	419	14.245	30.944	39.202	1.00	32.35	O
ATOM	2901	N	GLY	B	420	15.370	29.032	39.427	1.00	30.29	N
ATOM	2902	CA	GLY	B	420	15.091	28.621	38.065	1.00	27.83	C
ATOM	2903	C	GLY	B	420	15.930	29.299	36.980	1.00	24.88	C
ATOM	2904	O	GLY	B	420	16.843	30.054	37.303	1.00	24.54	O
ATOM	2905	N	PRO	B	421	15.617	29.068	35.694	1.00	26.97	N
ATOM	2906	CD	PRO	B	421	14.445	28.280	35.256	1.00	26.58	C
ATOM	2907	CA	PRO	B	421	16.320	29.631	34.534	1.00	26.79	C
ATOM	2908	CB	PRO	B	421	15.508	29.113	33.335	1.00	31.97	C
ATOM	2909	CG	PRO	B	421	14.810	27.921	33.845	1.00	32.59	C
ATOM	2910	C	PRO	B	421	16.400	31.148	34.507	1.00	31.93	C
ATOM	2911	O	PRO	B	421	15.430	31.851	34.801	1.00	26.82	O
ATOM	2912	N	LEU	B	422	17.570	31.643	34.112	1.00	24.30	N
ATOM	2913	CA	LEU	B	422	17.848	33.064	34.025	1.00	25.19	C
ATOM	2914	CB	LEU	B	422	19.316	33.263	33.632	1.00	26.63	C
ATOM	2915	CG	LEU	B	422	19.835	34.685	33.470	1.00	27.37	C
ATOM	2916	CD1	LEU	B	422	19.814	35.394	34.801	1.00	28.60	C
ATOM	2917	CD2	LEU	B	422	21.251	34.623	32.917	1.00	25.74	C
ATOM	2918	C	LEU	B	422	16.966	33.799	33.003	1.00	22.35	C
ATOM	2919	O	LEU	B	422	16.524	34.916	33.268	1.00	27.34	O
ATOM	2920	N	HIS	B	423	16.753	33.207	31.835	1.00	23.59	N
ATOM	2921	CA	HIS	B	423	15.944	33.884	30.829	1.00	33.17	C
ATOM	2922	CB	HIS	B	423	15.899	33.099	29.518	1.00	33.79	C
ATOM	2923	CG	HIS	B	423	15.322	31.725	29.650	1.00	30.44	C
ATOM	2924	CD2	HIS	B	423	15.309	30.856	30.688	1.00	33.89	C
ATOM	2925	ND1	HIS	B	423	14.631	31.109	28.626	1.00	40.96	N
ATOM	2926	CE1	HIS	B	423	14.222	29.919	29.029	1.00	35.92	C
ATOM	2927	NE2	HIS	B	423	14.621	29.740	30.276	1.00	37.97	N
ATOM	2928	C	HIS	B	423	14.525	34.142	31.341	1.00	37.06	C
ATOM	2929	O	HIS	B	423	13.989	35.236	31.153	1.00	39.39	O
ATOM	2930	N	LYS	B	424	13.927	33.149	31.995	1.00	28.98	N
ATOM	2931	CA	LYS	B	424	12.576	33.351	32.510	1.00	31.22	C
ATOM	2932	CB	LYS	B	424	11.957	32.006	32.883	1.00	28.63	C
ATOM	2933	CG	LYS	B	424	11.695	31.126	31.674	1.00	29.72	C
ATOM	2934	CD	LYS	B	424	11.076	29.800	32.117	1.00	42.69	C
ATOM	2935	CE	LYS	B	424	10.935	28.829	30.955	1.00	47.20	C
ATOM	2936	NZ	LYS	B	424	9.949	27.753	31.294	1.00	54.05	N
ATOM	2937	C	LYS	B	424	12.554	34.296	33.700	1.00	33.37	C
ATOM	2938	O	LYS	B	424	11.608	35.064	33.878	1.00	28.31	O
ATOM	2939	N	PHE	B	425	13.602	34.269	34.519	1.00	28.20	N
ATOM	2940	CA	PHE	B	425	13.660	35.137	35.681	1.00	26.95	C
ATOM	2941	CB	PHE	B	425	14.890	34.802	36.540	1.00	31.21	C
ATOM	2942	CG	PHE	B	425	15.042	35.680	37.747	1.00	32.76	C
ATOM	2943	CD1	PHE	B	425	14.318	35.431	38.904	1.00	41.67	C
ATOM	2944	CD2	PHE	B	425	15.886	36.782	37.710	1.00	35.66	C
ATOM	2945	CE1	PHE	B	425	14.429	36.272	40.011	1.00	40.79	C
ATOM	2946	CE2	PHE	B	425	16.010	37.631	38.805	1.00	43.64	C
ATOM	2947	CZ	PHE	B	425	15.277	37.377	39.962	1.00	45.58	C
ATOM	2948	C	PHE	B	425	13.713	36.629	35.310	1.00	28.99	C
ATOM	2949	O	PHE	B	425	13.149	37.468	36.010	1.00	28.02	O
ATOM	2950	N	LEU	B	426	14.379	36.961	34.212	1.00	27.54	N
ATOM	2951	CA	LEU	B	426	14.522	38.373	33.838	1.00	23.94	C
ATOM	2952	CB	LEU	B	426	15.838	38.577	33.072	1.00	25.46	C
ATOM	2953	CG	LEU	B	426	17.102	38.323	33.905	1.00	23.52	C
ATOM	2954	CD1	LEU	B	426	18.345	38.424	33.014	1.00	25.22	C

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ATOM   2955  CD2 LEU B 426     17.165  39.329  35.029  1.00  28.05      C
ATOM   2956  C   LEU B 426     13.368  38.959  33.019  1.00  28.74      C
ATOM   2957  O   LEU B 426     13.236  40.186  32.937  1.00  26.14      O
ATOM   2958  N   VAL B 427     12.553  38.100  32.415  1.00  27.70      N
ATOM   2959  CA  VAL B 427     11.442  38.584  31.583  1.00  30.96      C
ATOM   2960  CB  VAL B 427     10.577  37.409  31.059  1.00  35.17      C
ATOM   2961  CG1 VAL B 427      9.323  37.939  30.343  1.00  34.67      C
ATOM   2962  CG2 VAL B 427     11.391  36.561  30.082  1.00  31.17      C
ATOM   2963  C   VAL B 427     10.551  39.581  32.331  1.00  36.19      C
ATOM   2964  O   VAL B 427      9.984  39.269  33.386  1.00  37.99      O
ATOM   2965  N   GLY B 428     10.454  40.791  31.788  1.00  44.92      N
ATOM   2966  CA  GLY B 428      9.637  41.830  32.397  1.00  39.36      C
ATOM   2967  C   GLY B 428     10.144  42.432  33.696  1.00  46.68      C
ATOM   2968  O   GLY B 428      9.384  43.091  34.410  1.00  43.86      O
ATOM   2969  N   LYS B 429     11.419  42.231  34.019  1.00  36.36      N
ATOM   2970  CA  LYS B 429     11.960  42.772  35.258  1.00  41.33      C
ATOM   2971  CB  LYS B 429     12.561  41.638  36.086  1.00  45.43      C
ATOM   2972  CG  LYS B 429     11.519  40.599  36.492  1.00  48.96      C
ATOM   2973  CD  LYS B 429     11.975  39.804  37.699  1.00  53.23      C
ATOM   2974  CE  LYS B 429     11.004  38.680  38.025  1.00  52.24      C
ATOM   2975  NZ  LYS B 429     11.552  37.819  39.108  1.00  60.84      N
ATOM   2976  C   LYS B 429     12.990  43.880  35.028  1.00  42.92      C
ATOM   2977  O   LYS B 429     13.841  44.152  35.883  1.00  41.32      O
ATOM   2978  N   ARG B 430     12.889  44.535  33.878  1.00  38.04      N
ATOM   2979  CA  ARG B 430     13.824  45.594  33.532  1.00  50.47      C
ATOM   2980  CB  ARG B 430     13.541  46.091  32.116  1.00  52.47      C
ATOM   2981  CG  ARG B 430     14.669  46.918  31.520  1.00  63.31      C
ATOM   2982  CD  ARG B 430     14.548  47.014  29.999  1.00  63.30      C
ATOM   2983  NE  ARG B 430     15.857  46.896  29.351  1.00  63.29      N
ATOM   2984  CZ  ARG B 430     16.061  46.254  28.203  1.00  68.48      C
ATOM   2985  NH1 ARG B 430     15.043  45.680  27.573  1.00  63.45      N
ATOM   2986  NH2 ARG B 430     17.294  46.151  27.698  1.00  66.07      N
ATOM   2987  C   ARG B 430     13.774  46.754  34.518  1.00  53.77      C
ATOM   2988  O   ARG B 430     14.727  47.516  34.643  1.00  53.09      O
ATOM   2989  N   GLU B 431     12.661  46.879  35.235  1.00  54.55      N
ATOM   2990  CA  GLU B 431     12.518  47.959  36.196  1.00  55.49      C
ATOM   2991  CB  GLU B 431     11.167  48.658  36.020  1.00  57.64      C
ATOM   2992  CG  GLU B 431     11.104  49.556  34.797  1.00  61.36      C
ATOM   2993  CD  GLU B 431      9.932  50.515  34.839  1.00  66.74      C
ATOM   2994  OE1 GLU B 431      9.882  51.356  35.767  1.00  71.47      O
ATOM   2995  OE2 GLU B 431      9.062  50.433  33.946  1.00  68.60      O
ATOM   2996  C   GLU B 431     12.683  47.510  37.635  1.00  56.39      C
ATOM   2997  O   GLU B 431     12.608  48.325  38.550  1.00  57.92      O
ATOM   2998  N   GLU B 432     12.910  46.218  37.844  1.00  51.06      N
ATOM   2999  CA  GLU B 432     13.091  45.720  39.194  1.00  50.31      C
ATOM   3000  CB  GLU B 432     11.992  44.713  39.554  1.00  56.46      C
ATOM   3001  CG  GLU B 432     12.301  43.274  39.217  1.00  60.14      C
ATOM   3002  CD  GLU B 432     11.319  42.313  39.866  1.00  63.83      C
ATOM   3003  OE1 GLU B 432     10.118  42.375  39.526  1.00  66.40      O
ATOM   3004  OE2 GLU B 432     11.746  41.501  40.719  1.00  66.50      O
ATOM   3005  C   GLU B 432     14.464  45.083  39.364  1.00  49.21      C
ATOM   3006  O   GLU B 432     14.932  44.892  40.483  1.00  47.48      O
ATOM   3007  N   ILE B 433     15.111  44.756  38.246  1.00  43.34      N
ATOM   3008  CA  ILE B 433     16.442  44.156  38.288  1.00  35.43      C
ATOM   3009  CB  ILE B 433     16.436  42.734  37.688  1.00  40.48      C
ATOM   3010  CG2 ILE B 433     17.842  42.125  37.754  1.00  33.02      C
ATOM   3011  CG1 ILE B 433     15.463  41.850  38.460  1.00  39.44      C
ATOM   3012  CD1 ILE B 433     15.862  41.633  39.896  1.00  42.99      C
ATOM   3013  C   ILE B 433     17.335  45.049  37.446  1.00  37.58      C
ATOM   3014  O   ILE B 433     17.309  44.975  36.217  1.00  33.88      O
ATOM   3015  N   PRO B 434     18.125  45.919  38.097  1.00  33.22      N
ATOM   3016  CD  PRO B 434     18.093  46.179  39.546  1.00  39.68      C
ATOM   3017  CA  PRO B 434     19.038  46.857  37.435  1.00  37.36      C
ATOM   3018  CB  PRO B 434     19.661  47.606  38.614  1.00  36.58      C
ATOM   3019  CG  PRO B 434     18.559  47.616  39.604  1.00  47.33      C
ATOM   3020  C   PRO B 434     20.083  46.163  36.578  1.00  35.02      C
ATOM   3021  O   PRO B 434     20.382  44.986  36.785  1.00  29.87      O
ATOM   3022  N   VAL B 435     20.644  46.904  35.625  1.00  30.90      N
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ATOM   3023  CA   VAL B 435     21.669  46.349  34.750  1.00  33.32           C
ATOM   3024  CB   VAL B 435     22.138  47.391  33.699  1.00  32.31           C
ATOM   3025  CG1  VAL B 435     23.255  46.802  32.839  1.00  32.23           C
ATOM   3026  CG2  VAL B 435     20.968  47.792  32.821  1.00  38.32           C
ATOM   3027  C    VAL B 435     22.862  45.875  35.570  1.00  31.88           C
ATOM   3028  O    VAL B 435     23.504  44.873  35.218  1.00  26.54           O
ATOM   3029  N    SER B 436     23.165  46.593  36.652  1.00  28.96           N
ATOM   3030  CA   SER B 436     24.278  46.225  37.519  1.00  29.85           C
ATOM   3031  CB   SER B 436     24.437  47.262  38.646  1.00  33.71           C
ATOM   3032  OG   SER B 436     23.246  47.361  39.414  1.00  36.37           O
ATOM   3033  C    SER B 436     24.077  44.815  38.112  1.00  30.64           C
ATOM   3034  O    SER B 436     25.039  44.069  38.281  1.00  28.51           O
ATOM   3035  N    ASN B 437     22.832  44.464  38.426  1.00  25.41           N
ATOM   3036  CA   ASN B 437     22.502  43.155  38.993  1.00  26.86           C
ATOM   3037  CB   ASN B 437     21.088  43.219  39.581  1.00  29.47           C
ATOM   3038  CG   ASN B 437     20.692  41.975  40.391  1.00  32.65           C
ATOM   3039  OD1  ASN B 437     19.669  41.997  41.081  1.00  33.91           O
ATOM   3040  ND2  ASN B 437     21.466  40.891  40.294  1.00  29.62           N
ATOM   3041  C    ASN B 437     22.632  42.121  37.858  1.00  26.75           C
ATOM   3042  O    ASN B 437     23.126  41.010  38.070  1.00  26.10           O
ATOM   3043  N    VAL B 438     22.220  42.483  36.648  1.00  26.29           N
ATOM   3044  CA   VAL B 438     22.390  41.546  35.548  1.00  22.79           C
ATOM   3045  CB   VAL B 438     21.761  42.073  34.250  1.00  26.63           C
ATOM   3046  CG1  VAL B 438     22.085  41.136  33.099  1.00  25.60           C
ATOM   3047  CG2  VAL B 438     20.231  42.187  34.428  1.00  27.00           C
ATOM   3048  C    VAL B 438     23.896  41.313  35.343  1.00  25.06           C
ATOM   3049  O    VAL B 438     24.325  40.178  35.172  1.00  22.07           O
ATOM   3050  N    ALA B 439     24.704  42.383  35.376  1.00  23.57           N
ATOM   3051  CA   ALA B 439     26.156  42.223  35.206  1.00  24.57           C
ATOM   3052  CB   ALA B 439     26.858  43.623  35.135  1.00  23.14           C
ATOM   3053  C    ALA B 439     26.775  41.369  36.326  1.00  21.99           C
ATOM   3054  O    ALA B 439     27.724  40.622  36.086  1.00  23.36           O
ATOM   3055  N    GLU B 440     26.225  41.467  37.540  1.00  22.47           N
ATOM   3056  CA   GLU B 440     26.729  40.684  38.660  1.00  26.63           C
ATOM   3057  CB   GLU B 440     25.946  41.027  39.937  1.00  28.89           C
ATOM   3058  CG   GLU B 440     26.220  40.080  41.109  1.00  27.35           C
ATOM   3059  CD   GLU B 440     25.304  40.355  42.295  1.00  39.88           C
ATOM   3060  OE1  GLU B 440     24.142  40.766  42.075  1.00  37.76           O
ATOM   3061  OE2  GLU B 440     25.750  40.145  43.445  1.00  37.86           O
ATOM   3062  C    GLU B 440     26.575  39.190  38.331  1.00  28.92           C
ATOM   3063  O    GLU B 440     27.503  38.411  38.506  1.00  22.24           O
ATOM   3064  N    LEU B 441     25.393  38.812  37.848  1.00  22.17           N
ATOM   3065  CA   LEU B 441     25.086  37.423  37.488  1.00  22.51           C
ATOM   3066  CB   LEU B 441     23.590  37.301  37.148  1.00  22.22           C
ATOM   3067  CG   LEU B 441     22.647  37.692  38.290  1.00  26.11           C
ATOM   3068  CD1  LEU B 441     21.191  37.675  37.823  1.00  26.08           C
ATOM   3069  CD2  LEU B 441     22.853  36.702  39.443  1.00  23.20           C
ATOM   3070  C    LEU B 441     25.930  36.973  36.296  1.00  20.83           C
ATOM   3071  O    LEU B 441     26.449  35.848  36.280  1.00  22.40           O
ATOM   3072  N    LEU B 442     26.062  37.829  35.290  1.00  20.51           N
ATOM   3073  CA   LEU B 442     26.893  37.442  34.147  1.00  24.46           C
ATOM   3074  CB   LEU B 442     26.822  38.487  33.038  1.00  22.94           C
ATOM   3075  CG   LEU B 442     25.484  38.527  32.291  1.00  21.56           C
ATOM   3076  CD1  LEU B 442     25.459  39.693  31.263  1.00  24.52           C
ATOM   3077  CD2  LEU B 442     25.268  37.168  31.601  1.00  22.91           C
ATOM   3078  C    LEU B 442     28.346  37.244  34.590  1.00  21.94           C
ATOM   3079  O    LEU B 442     29.033  36.352  34.105  1.00  22.31           O
ATOM   3080  N    HIS B 443     28.811  38.055  35.530  1.00  20.83           N
ATOM   3081  CA   HIS B 443     30.193  37.888  35.998  1.00  21.14           C
ATOM   3082  CB   HIS B 443     30.598  39.048  36.918  1.00  25.52           C
ATOM   3083  CG   HIS B 443     31.965  38.875  37.502  1.00  27.68           C
ATOM   3084  CD2  HIS B 443     33.143  38.507  36.932  1.00  25.68           C
ATOM   3085  ND1  HIS B 443     32.210  38.987  38.855  1.00  26.29           N
ATOM   3086  CE1  HIS B 443     33.476  38.691  39.096  1.00  24.28           C
ATOM   3087  NE2  HIS B 443     34.064  38.394  37.947  1.00  23.65           N
ATOM   3088  C    HIS B 443     30.367  36.530  36.715  1.00  22.96           C
ATOM   3089  O    HIS B 443     31.374  35.841  36.541  1.00  21.47           O
ATOM   3090  N    GLN B 444     29.370  36.130  37.498  1.00  22.87           N
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ATOM	3091	CA	GLN	B	444	29.429	34.843	38.177	1.00	19.38	C
ATOM	3092	CB	GLN	B	444	28.203	34.688	39.080	1.00	21.91	C
ATOM	3093	CG	GLN	B	444	28.254	35.697	40.221	1.00	22.66	C
ATOM	3094	CD	GLN	B	444	27.013	35.648	41.058	1.00	25.66	C
ATOM	3095	OE1	GLN	B	444	25.994	35.130	40.633	1.00	27.50	O
ATOM	3096	NE2	GLN	B	444	27.089	36.206	42.258	1.00	27.58	N
ATOM	3097	C	GLN	B	444	29.483	33.735	37.149	1.00	22.05	C
ATOM	3098	O	GLN	B	444	30.248	32.792	37.288	1.00	23.64	O
ATOM	3099	N	VAL	B	445	28.691	33.867	36.089	1.00	20.47	N
ATOM	3100	CA	VAL	B	445	28.735	32.863	35.044	1.00	19.55	C
ATOM	3101	CB	VAL	B	445	27.705	33.147	33.926	1.00	20.65	C
ATOM	3102	CG1	VAL	B	445	27.876	32.121	32.784	1.00	21.65	C
ATOM	3103	CG2	VAL	B	445	26.300	33.049	34.493	1.00	21.06	C
ATOM	3104	C	VAL	B	445	30.151	32.857	34.435	1.00	21.63	C
ATOM	3105	O	VAL	B	445	30.682	31.792	34.150	1.00	21.53	O
ATOM	3106	N	SER	B	446	30.757	34.031	34.251	1.00	19.30	N
ATOM	3107	CA	SER	B	446	32.108	34.047	33.663	1.00	22.00	C
ATOM	3108	CB	SER	B	446	32.570	35.480	33.292	1.00	19.55	C
ATOM	3109	OG	SER	B	446	32.902	36.261	34.407	1.00	22.80	O
ATOM	3110	C	SER	B	446	33.142	33.399	34.600	1.00	22.37	C
ATOM	3111	O	SER	B	446	34.109	32.812	34.131	1.00	21.37	O
ATOM	3112	N	MET	B	447	32.925	33.497	35.909	1.00	20.23	N
ATOM	3113	CA	MET	B	447	33.860	32.859	36.846	1.00	24.29	C
ATOM	3114	CB	MET	B	447	33.640	33.376	38.272	1.00	23.41	C
ATOM	3115	CG	MET	B	447	34.123	34.806	38.446	1.00	27.21	C
ATOM	3116	SD	MET	B	447	34.087	35.327	40.218	1.00	29.84	S
ATOM	3117	CE	MET	B	447	32.347	35.711	40.421	1.00	28.71	C
ATOM	3118	C	MET	B	447	33.698	31.342	36.767	1.00	24.03	C
ATOM	3119	O	MET	B	447	34.681	30.617	36.778	1.00	23.04	O
ATOM	3120	N	GLY	B	448	32.460	30.858	36.669	1.00	19.35	N
ATOM	3121	CA	GLY	B	448	32.276	29.423	36.546	1.00	21.93	C
ATOM	3122	C	GLY	B	448	32.898	28.922	35.248	1.00	28.63	C
ATOM	3123	O	GLY	B	448	33.506	27.847	35.242	1.00	23.12	O
ATOM	3124	N	MET	B	449	32.758	29.687	34.155	1.00	21.69	N
ATOM	3125	CA	MET	B	449	33.325	29.240	32.866	1.00	20.45	C
ATOM	3126	CB	MET	B	449	32.714	30.027	31.692	1.00	22.80	C
ATOM	3127	CG	MET	B	449	31.201	29.789	31.468	1.00	21.04	C
ATOM	3128	SD	MET	B	449	30.734	28.035	31.300	1.00	25.98	S
ATOM	3129	CE	MET	B	449	31.656	27.593	29.836	1.00	24.75	C
ATOM	3130	C	MET	B	449	34.852	29.343	32.825	1.00	19.20	C
ATOM	3131	O	MET	B	449	35.526	28.532	32.182	1.00	23.26	O
ATOM	3132	N	LYS	B	450	35.399	30.330	33.520	1.00	21.31	N
ATOM	3133	CA	LYS	B	450	36.847	30.477	33.578	1.00	22.27	C
ATOM	3134	CB	LYS	B	450	37.188	31.710	34.397	1.00	25.65	C
ATOM	3135	CG	LYS	B	450	38.686	31.870	34.602	1.00	35.16	C
ATOM	3136	CD	LYS	B	450	38.967	32.940	35.604	1.00	39.35	C
ATOM	3137	CE	LYS	B	450	40.432	32.855	36.005	1.00	41.39	C
ATOM	3138	NZ	LYS	B	450	40.770	33.998	36.884	1.00	50.53	N
ATOM	3139	C	LYS	B	450	37.382	29.201	34.259	1.00	21.58	C
ATOM	3140	O	LYS	B	450	38.394	28.634	33.863	1.00	23.54	O
ATOM	3141	N	TYR	B	451	36.667	28.738	35.272	1.00	22.85	N
ATOM	3142	CA	TYR	B	451	37.061	27.508	35.980	1.00	26.56	C
ATOM	3143	CB	TYR	B	451	36.179	27.307	37.225	1.00	31.08	C
ATOM	3144	CG	TYR	B	451	36.420	25.996	37.963	1.00	26.37	C
ATOM	3145	CD1	TYR	B	451	37.523	25.831	38.813	1.00	32.42	C
ATOM	3146	CE1	TYR	B	451	37.719	24.612	39.503	1.00	35.50	C
ATOM	3147	CD2	TYR	B	451	35.543	24.934	37.810	1.00	29.25	C
ATOM	3148	CE2	TYR	B	451	35.737	23.731	38.458	1.00	36.41	C
ATOM	3149	CZ	TYR	B	451	36.814	23.570	39.307	1.00	36.89	C
ATOM	3150	OH	TYR	B	451	36.928	22.357	39.947	1.00	35.03	O
ATOM	3151	C	TYR	B	451	36.975	26.290	35.084	1.00	23.27	C
ATOM	3152	O	TYR	B	451	37.904	25.484	35.035	1.00	22.89	O
ATOM	3153	N	LEU	B	452	35.881	26.144	34.339	1.00	21.39	N
ATOM	3154	CA	LEU	B	452	35.757	25.005	33.457	1.00	21.19	C
ATOM	3155	CB	LEU	B	452	34.379	24.995	32.735	1.00	25.34	C
ATOM	3156	CG	LEU	B	452	33.197	24.695	33.653	1.00	31.38	C
ATOM	3157	CD1	LEU	B	452	31.922	24.872	32.832	1.00	39.34	C
ATOM	3158	CD2	LEU	B	452	33.275	23.271	34.196	1.00	34.35	C

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ATOM	3159	C	LEU	B	452	36.855	24.995	32.417	1.00	23.04
ATOM	3160	O	LEU	B	452	37.399	23.930	32.098	1.00	23.98
ATOM	3161	N	GLU	B	453	37.178	26.179	31.894	1.00	21.93
ATOM	3162	CA	GLU	B	453	38.215	26.298	30.881	1.00	24.62
ATOM	3163	CB	GLU	B	453	38.283	27.747	30.398	1.00	25.46
ATOM	3164	CG	GLU	B	453	39.415	28.050	29.406	1.00	28.82
ATOM	3165	CD	GLU	B	453	39.405	29.510	28.934	1.00	36.37
ATOM	3166	OE1	GLU	B	453	40.016	30.376	29.621	1.00	33.79
ATOM	3167	OE2	GLU	B	453	38.776	29.790	27.880	1.00	31.16
ATOM	3168	C	GLU	B	453	39.585	25.865	31.454	1.00	25.13
ATOM	3169	O	GLU	B	453	40.345	25.115	30.812	1.00	25.39
ATOM	3170	N	GLU	B	454	39.908	26.351	32.645	1.00	22.62
ATOM	3171	CA	GLU	B	454	41.204	25.996	33.245	1.00	26.22
ATOM	3172	CB	GLU	B	454	41.436	26.762	34.552	1.00	30.29
ATOM	3173	CG	GLU	B	454	40.519	26.379	35.681	1.00	43.54
ATOM	3174	CD	GLU	B	454	40.821	27.144	36.972	1.00	58.22
ATOM	3175	OE1	GLU	B	454	40.838	28.404	36.941	1.00	50.28
ATOM	3176	OE2	GLU	B	454	41.029	26.480	38.019	1.00	56.54
ATOM	3177	C	GLU	B	454	41.284	24.501	33.507	1.00	32.56
ATOM	3178	O	GLU	B	454	42.368	23.927	33.489	1.00	31.49
ATOM	3179	N	LYS	B	455	40.147	23.852	33.728	1.00	26.00
ATOM	3180	CA	LYS	B	455	40.141	22.406	33.979	1.00	27.14
ATOM	3181	CB	LYS	B	455	39.043	22.032	34.991	1.00	26.60
ATOM	3182	CG	LYS	B	455	39.173	22.743	36.346	1.00	29.96
ATOM	3183	CD	LYS	B	455	40.493	22.365	37.009	1.00	36.01
ATOM	3184	CE	LYS	B	455	40.733	23.118	38.322	1.00	40.11
ATOM	3185	NZ	LYS	B	455	42.067	22.747	38.909	1.00	33.10
ATOM	3186	C	LYS	B	455	39.954	21.605	32.692	1.00	26.89
ATOM	3187	O	LYS	B	455	39.757	20.397	32.732	1.00	31.85
ATOM	3188	N	ASN	B	456	40.047	22.280	31.551	1.00	27.82
ATOM	3189	CA	ASN	B	456	39.901	21.640	30.245	1.00	30.31
ATOM	3190	CB	ASN	B	456	41.089	20.707	29.967	1.00	32.92
ATOM	3191	CG	ASN	B	456	42.384	21.456	29.907	1.00	40.95
ATOM	3192	OD1	ASN	B	456	42.556	22.351	29.081	1.00	37.33
ATOM	3193	ND2	ASN	B	456	43.313	21.110	30.803	1.00	43.15
ATOM	3194	C	ASN	B	456	38.602	20.891	29.992	1.00	30.21
ATOM	3195	O	ASN	B	456	38.614	19.772	29.473	1.00	28.50
ATOM	3196	N	PHE	B	457	37.482	21.494	30.381	1.00	25.11
ATOM	3197	CA	PHE	B	457	36.193	20.899	30.098	1.00	22.51
ATOM	3198	CB	PHE	B	457	35.376	20.679	31.386	1.00	23.31
ATOM	3199	CG	PHE	B	457	35.848	19.515	32.204	1.00	26.75
ATOM	3200	CD1	PHE	B	457	36.692	19.706	33.302	1.00	38.60
ATOM	3201	CD2	PHE	B	457	35.456	18.232	31.877	1.00	29.58
ATOM	3202	CE1	PHE	B	457	37.125	18.614	34.055	1.00	40.07
ATOM	3203	CE2	PHE	B	457	35.887	17.140	32.624	1.00	35.33
ATOM	3204	CZ	PHE	B	457	36.718	17.334	33.710	1.00	29.78
ATOM	3205	C	PHE	B	457	35.435	21.903	29.198	1.00	20.08
ATOM	3206	O	PHE	B	457	35.555	23.105	29.396	1.00	24.84
ATOM	3207	N	VAL	B	458	34.657	21.370	28.247	1.00	22.46
ATOM	3208	CA	VAL	B	458	33.832	22.189	27.351	1.00	19.50
ATOM	3209	CB	VAL	B	458	34.039	21.771	25.864	1.00	24.51
ATOM	3210	CG1	VAL	B	458	33.044	22.521	24.946	1.00	20.39
ATOM	3211	CG2	VAL	B	458	35.451	22.094	25.438	1.00	26.69
ATOM	3212	C	VAL	B	458	32.365	21.908	27.749	1.00	22.31
ATOM	3213	O	VAL	B	458	31.956	20.779	27.818	1.00	23.69
ATOM	3214	N	HIS	B	459	31.581	22.946	27.977	1.00	21.21
ATOM	3215	CA	HIS	B	459	30.176	22.720	28.415	1.00	20.87
ATOM	3216	CB	HIS	B	459	29.670	23.998	29.119	1.00	26.99
ATOM	3217	CG	HIS	B	459	28.294	23.866	29.693	1.00	26.79
ATOM	3218	CD2	HIS	B	459	27.869	23.814	30.978	1.00	33.82
ATOM	3219	ND1	HIS	B	459	27.163	23.762	28.912	1.00	30.62
ATOM	3220	CE1	HIS	B	459	26.099	23.665	29.691	1.00	28.63
ATOM	3221	NE2	HIS	B	459	26.500	23.693	30.949	1.00	26.47
ATOM	3222	C	HIS	B	459	29.279	22.376	27.225	1.00	22.74
ATOM	3223	O	HIS	B	459	28.472	21.409	27.260	1.00	26.21
ATOM	3224	N	ARG	B	460	29.432	23.186	26.178	1.00	23.74
ATOM	3225	CA	ARG	B	460	28.716	23.083	24.911	1.00	23.96
ATOM	3226	CB	ARG	B	460	28.766	21.644	24.390	1.00	27.31

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ATOM	3227	CG	ARG	B	460	28.259	21.546	22.972	1.00	37.56	C
ATOM	3228	CD	ARG	B	460	28.279	20.147	22.427	1.00	32.14	C
ATOM	3229	NE	ARG	B	460	27.254	20.032	21.406	1.00	31.71	N
ATOM	3230	CZ	ARG	B	460	27.008	18.927	20.699	1.00	39.03	C
ATOM	3231	NH1	ARG	B	460	27.721	17.830	20.903	1.00	34.17	N
ATOM	3232	NH2	ARG	B	460	26.040	18.924	19.793	1.00	42.19	N
ATOM	3233	C	ARG	B	460	27.261	23.562	24.895	1.00	30.30	C
ATOM	3234	O	ARG	B	460	26.726	23.888	23.833	1.00	37.44	O
ATOM	3235	N	ASP	B	461	26.628	23.648	26.054	1.00	24.84	N
ATOM	3236	CA	ASP	B	461	25.230	24.057	26.087	1.00	27.22	C
ATOM	3237	CB	ASP	B	461	24.389	22.843	26.547	1.00	29.93	C
ATOM	3238	CG	ASP	B	461	22.893	22.954	26.185	1.00	40.58	C
ATOM	3239	OD1	ASP	B	461	22.497	23.822	25.374	1.00	47.29	O
ATOM	3240	OD2	ASP	B	461	22.100	22.138	26.718	1.00	51.22	O
ATOM	3241	C	ASP	B	461	25.039	25.281	26.998	1.00	27.48	C
ATOM	3242	O	ASP	B	461	24.054	25.401	27.713	1.00	25.86	O
ATOM	3243	N	LEU	B	462	25.985	26.210	26.963	1.00	21.15	N
ATOM	3244	CA	LEU	B	462	25.841	27.399	27.788	1.00	20.41	C
ATOM	3245	CB	LEU	B	462	27.200	28.106	27.940	1.00	22.91	C
ATOM	3246	CG	LEU	B	462	27.216	29.380	28.792	1.00	28.71	C
ATOM	3247	CD1	LEU	B	462	26.774	29.008	30.203	1.00	30.96	C
ATOM	3248	CD2	LEU	B	462	28.614	30.037	28.792	1.00	27.89	C
ATOM	3249	C	LEU	B	462	24.790	28.300	27.113	1.00	25.32	C
ATOM	3250	O	LEU	B	462	24.913	28.640	25.958	1.00	27.45	O
ATOM	3251	N	ALA	B	463	23.737	28.637	27.847	1.00	20.92	N
ATOM	3252	CA	ALA	B	463	22.645	29.482	27.350	1.00	20.29	C
ATOM	3253	CB	ALA	B	463	21.709	28.658	26.431	1.00	17.73	C
ATOM	3254	C	ALA	B	463	21.905	29.962	28.596	1.00	21.81	C
ATOM	3255	O	ALA	B	463	21.978	29.319	29.655	1.00	21.64	O
ATOM	3256	N	ALA	B	464	21.187	31.069	28.492	1.00	19.40	N
ATOM	3257	CA	ALA	B	464	20.510	31.586	29.655	1.00	21.46	C
ATOM	3258	CB	ALA	B	464	19.750	32.879	29.294	1.00	20.54	C
ATOM	3259	C	ALA	B	464	19.567	30.560	30.288	1.00	23.11	C
ATOM	3260	O	ALA	B	464	19.399	30.567	31.499	1.00	22.21	O
ATOM	3261	N	ARG	B	465	18.963	29.703	29.468	1.00	22.19	N
ATOM	3262	CA	ARG	B	465	18.036	28.679	29.955	1.00	25.34	C
ATOM	3263	CB	ARG	B	465	17.372	27.947	28.783	1.00	22.79	C
ATOM	3264	CG	ARG	B	465	18.310	27.131	27.897	1.00	21.09	C
ATOM	3265	CD	ARG	B	465	17.586	26.576	26.650	1.00	28.36	C
ATOM	3266	NE	ARG	B	465	18.537	25.936	25.752	1.00	33.20	N
ATOM	3267	CZ	ARG	B	465	19.230	26.568	24.801	1.00	41.11	C
ATOM	3268	NH1	ARG	B	465	19.074	27.873	24.592	1.00	34.56	N
ATOM	3269	NH2	ARG	B	465	20.129	25.908	24.099	1.00	36.89	N
ATOM	3270	C	ARG	B	465	18.746	27.650	30.840	1.00	27.21	C
ATOM	3271	O	ARG	B	465	18.098	26.930	31.600	1.00	25.31	O
ATOM	3272	N	ASN	B	466	20.075	27.583	30.727	1.00	26.22	N
ATOM	3273	CA	ASN	B	466	20.851	26.640	31.535	1.00	22.74	C
ATOM	3274	CB	ASN	B	466	21.777	25.809	30.647	1.00	20.44	C
ATOM	3275	CG	ASN	B	466	21.022	24.810	29.806	1.00	31.49	C
ATOM	3276	OD1	ASN	B	466	19.963	24.316	30.217	1.00	26.09	O
ATOM	3277	ND2	ASN	B	466	21.556	24.496	28.624	1.00	25.81	N
ATOM	3278	C	ASN	B	466	21.608	27.277	32.677	1.00	24.14	C
ATOM	3279	O	ASN	B	466	22.379	26.617	33.372	1.00	25.61	O
ATOM	3280	N	VAL	B	467	21.384	28.563	32.895	1.00	19.90	N
ATOM	3281	CA	VAL	B	467	21.999	29.239	34.013	1.00	18.65	C
ATOM	3282	CB	VAL	B	467	22.443	30.652	33.640	1.00	21.94	C
ATOM	3283	CG1	VAL	B	467	22.840	31.414	34.910	1.00	20.29	C
ATOM	3284	CG2	VAL	B	467	23.617	30.565	32.634	1.00	21.43	C
ATOM	3285	C	VAL	B	467	20.834	29.323	35.002	1.00	25.03	C
ATOM	3286	O	VAL	B	467	19.757	29.829	34.659	1.00	24.55	O
ATOM	3287	N	LEU	B	468	21.047	28.821	36.212	1.00	21.56	N
ATOM	3288	CA	LEU	B	468	19.972	28.813	37.219	1.00	22.81	C
ATOM	3289	CB	LEU	B	468	19.738	27.385	37.734	1.00	22.41	C
ATOM	3290	CG	LEU	B	468	19.493	26.291	36.695	1.00	25.80	C
ATOM	3291	CD1	LEU	B	468	19.568	24.927	37.347	1.00	27.13	C
ATOM	3292	CD2	LEU	B	468	18.128	26.521	36.038	1.00	28.96	C
ATOM	3293	C	LEU	B	468	20.287	29.707	38.394	1.00	27.22	C
ATOM	3294	O	LEU	B	468	21.426	29.782	38.826	1.00	26.70	O

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ATOM	3295	N	LEU	B	469	19.262	30.349	38.960	1.00	24.32	N
ATOM	3296	CA	LEU	B	469	19.511	31.234	40.078	1.00	23.08	C
ATOM	3297	CB	LEU	B	469	18.687	32.498	39.908	1.00	24.42	C
ATOM	3298	CG	LEU	B	469	18.985	33.232	38.596	1.00	37.62	C
ATOM	3299	CD1	LEU	B	469	17.999	34.336	38.412	1.00	40.80	C
ATOM	3300	CD2	LEU	B	469	20.384	33.797	38.612	1.00	33.91	C
ATOM	3301	C	LEU	B	469	19.216	30.625	41.440	1.00	26.89	C
ATOM	3302	O	LEU	B	469	18.162	30.024	41.643	1.00	27.22	O
ATOM	3303	N	VAL	B	470	20.154	30.766	42.366	1.00	27.63	N
ATOM	3304	CA	VAL	B	470	19.903	30.311	43.718	1.00	30.31	C
ATOM	3305	CB	VAL	B	470	21.199	30.132	44.520	1.00	33.68	C
ATOM	3306	CG1	VAL	B	470	20.862	29.797	45.973	1.00	34.34	C
ATOM	3307	CG2	VAL	B	470	22.027	29.002	43.912	1.00	28.72	C
ATOM	3308	C	VAL	B	470	19.057	31.450	44.300	1.00	31.84	C
ATOM	3309	O	VAL	B	470	18.096	31.210	45.051	1.00	33.69	O
ATOM	3310	N	ASN	B	471	19.407	32.682	43.930	1.00	29.94	N
ATOM	3311	CA	ASN	B	471	18.688	33.903	44.335	1.00	34.01	C
ATOM	3312	CB	ASN	B	471	19.139	34.394	45.723	1.00	38.51	C
ATOM	3313	CG	ASN	B	471	20.631	34.554	45.824	1.00	41.61	C
ATOM	3314	OD1	ASN	B	471	21.336	33.627	46.225	1.00	62.13	O
ATOM	3315	ND2	ASN	B	471	21.129	35.710	45.433	1.00	34.16	N
ATOM	3316	C	ASN	B	471	19.009	34.971	43.283	1.00	32.05	C
ATOM	3317	O	ASN	B	471	19.796	34.712	42.378	1.00	29.59	O
ATOM	3318	N	ARG	B	472	18.434	36.170	43.395	1.00	31.13	N
ATOM	3319	CA	ARG	B	472	18.687	37.216	42.392	1.00	33.64	C
ATOM	3320	CB	ARG	B	472	17.766	38.417	42.631	1.00	35.84	C
ATOM	3321	CG	ARG	B	472	18.042	39.147	43.924	1.00	37.87	C
ATOM	3322	CD	ARG	B	472	17.142	40.371	44.053	1.00	40.99	C
ATOM	3323	NE	ARG	B	472	17.621	41.483	43.240	1.00	43.11	N
ATOM	3324	CZ	ARG	B	472	16.972	42.633	43.074	1.00	48.70	C
ATOM	3325	NH1	ARG	B	472	15.795	42.832	43.667	1.00	41.99	N
ATOM	3326	NH2	ARG	B	472	17.503	43.593	42.334	1.00	44.48	N
ATOM	3327	C	ARG	B	472	20.132	37.702	42.324	1.00	24.49	C
ATOM	3328	O	ARG	B	472	20.492	38.446	41.423	1.00	30.50	O
ATOM	3329	N	HIS	B	473	20.952	37.294	43.288	1.00	26.54	N
ATOM	3330	CA	HIS	B	473	22.340	37.700	43.324	1.00	30.93	C
ATOM	3331	CB	HIS	B	473	22.628	38.517	44.614	1.00	28.14	C
ATOM	3332	CG	HIS	B	473	21.888	39.817	44.673	1.00	32.49	C
ATOM	3333	CD2	HIS	B	473	20.856	40.225	45.451	1.00	40.34	C
ATOM	3334	ND1	HIS	B	473	22.125	40.845	43.786	1.00	36.03	N
ATOM	3335	CE1	HIS	B	473	21.266	41.825	44.008	1.00	41.10	C
ATOM	3336	NE2	HIS	B	473	20.482	41.473	45.013	1.00	42.57	N
ATOM	3337	C	HIS	B	473	23.276	36.497	43.260	1.00	25.86	C
ATOM	3338	O	HIS	B	473	24.472	36.628	43.573	1.00	25.18	O
ATOM	3339	N	TYR	B	474	22.760	35.337	42.854	1.00	26.93	N
ATOM	3340	CA	TYR	B	474	23.614	34.141	42.810	1.00	28.61	C
ATOM	3341	CB	TYR	B	474	23.597	33.447	44.184	1.00	26.00	C
ATOM	3342	CG	TYR	B	474	24.589	32.302	44.396	1.00	29.87	C
ATOM	3343	CD1	TYR	B	474	25.645	32.050	43.505	1.00	27.42	C
ATOM	3344	CE1	TYR	B	474	26.563	30.995	43.747	1.00	31.28	C
ATOM	3345	CD2	TYR	B	474	24.477	31.481	45.523	1.00	34.24	C
ATOM	3346	CE2	TYR	B	474	25.377	30.444	45.768	1.00	37.06	C
ATOM	3347	CZ	TYR	B	474	26.416	30.198	44.888	1.00	35.99	C
ATOM	3348	OH	TYR	B	474	27.285	29.160	45.187	1.00	32.29	O
ATOM	3349	C	TYR	B	474	23.218	33.160	41.719	1.00	27.49	C
ATOM	3350	O	TYR	B	474	22.237	32.413	41.862	1.00	27.72	O
ATOM	3351	N	ALA	B	475	24.003	33.153	40.638	1.00	21.66	N
ATOM	3352	CA	ALA	B	475	23.744	32.279	39.509	1.00	25.73	C
ATOM	3353	CB	ALA	B	475	23.886	33.075	38.200	1.00	27.00	C
ATOM	3354	C	ALA	B	475	24.680	31.057	39.486	1.00	25.53	C
ATOM	3355	O	ALA	B	475	25.809	31.113	39.970	1.00	26.97	O
ATOM	3356	N	LYS	B	476	24.190	29.953	38.921	1.00	22.58	N
ATOM	3357	CA	LYS	B	476	24.987	28.739	38.771	1.00	23.46	C
ATOM	3358	CB	LYS	B	476	24.594	27.691	39.834	1.00	24.43	C
ATOM	3359	CG	LYS	B	476	25.144	28.000	41.221	1.00	25.55	C
ATOM	3360	CD	LYS	B	476	24.578	26.972	42.233	1.00	32.01	C
ATOM	3361	CE	LYS	B	476	25.288	27.036	43.577	1.00	36.59	C
ATOM	3362	NZ	LYS	B	476	26.553	26.248	43.526	1.00	37.14	N

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ATOM	3363	C	LYS	B	476	24.787	28.124	37.402	1.00	24.32	C
ATOM	3364	O	LYS	B	476	23.658	28.084	36.876	1.00	24.88	O
ATOM	3365	N	ILE	B	477	25.869	27.620	36.815	1.00	21.48	N
ATOM	3366	CA	ILE	B	477	25.778	26.980	35.511	1.00	23.09	C
ATOM	3367	CB	ILE	B	477	27.139	26.937	34.843	1.00	20.87	C
ATOM	3368	CG2	ILE	B	477	27.065	26.129	33.544	1.00	24.48	C
ATOM	3369	CG1	ILE	B	477	27.644	28.370	34.642	1.00	22.01	C
ATOM	3370	CD1	ILE	B	477	29.143	28.461	34.443	1.00	23.58	C
ATOM	3371	C	ILE	B	477	25.297	25.560	35.689	1.00	26.88	C
ATOM	3372	O	ILE	B	477	25.794	24.860	36.565	1.00	24.82	O
ATOM	3373	N	SER	B	478	24.351	25.111	34.855	1.00	22.63	N
ATOM	3374	CA	SER	B	478	23.876	23.743	34.992	1.00	23.59	C
ATOM	3375	CB	SER	B	478	22.474	23.741	35.578	1.00	30.50	C
ATOM	3376	OG	SER	B	478	21.607	24.274	34.601	1.00	40.13	O
ATOM	3377	C	SER	B	478	23.842	22.996	33.664	1.00	27.84	C
ATOM	3378	O	SER	B	478	24.253	23.528	32.616	1.00	27.42	O
ATOM	3379	N	ASP	B	479	23.302	21.775	33.730	1.00	23.72	N
ATOM	3380	CA	ASP	B	479	23.164	20.821	32.611	1.00	25.82	C
ATOM	3381	CB	ASP	B	479	22.094	21.256	31.585	1.00	24.35	C
ATOM	3382	CG	ASP	B	479	21.711	20.104	30.636	1.00	34.90	C
ATOM	3383	OD1	ASP	B	479	22.419	19.076	30.636	1.00	30.23	O
ATOM	3384	OD2	ASP	B	479	20.703	20.214	29.899	1.00	30.91	O
ATOM	3385	C	ASP	B	479	24.460	20.489	31.878	1.00	24.50	C
ATOM	3386	O	ASP	B	479	24.751	21.037	30.784	1.00	21.34	O
ATOM	3387	N	PHE	B	480	25.197	19.529	32.444	1.00	26.62	N
ATOM	3388	CA	PHE	B	480	26.464	19.062	31.863	1.00	27.44	C
ATOM	3389	CB	PHE	B	480	27.474	18.812	32.993	1.00	26.01	C
ATOM	3390	CG	PHE	B	480	27.893	20.075	33.696	1.00	25.53	C
ATOM	3391	CD1	PHE	B	480	29.029	20.788	33.289	1.00	37.11	C
ATOM	3392	CD2	PHE	B	480	27.095	20.617	34.700	1.00	30.32	C
ATOM	3393	CE1	PHE	B	480	29.346	22.023	33.870	1.00	34.94	C
ATOM	3394	CE2	PHE	B	480	27.403	21.850	35.279	1.00	31.64	C
ATOM	3395	CZ	PHE	B	480	28.520	22.555	34.866	1.00	33.32	C
ATOM	3396	C	PHE	B	480	26.288	17.810	30.989	1.00	23.32	C
ATOM	3397	O	PHE	B	480	27.242	17.078	30.712	1.00	29.60	O
ATOM	3398	N	GLY	B	481	25.059	17.586	30.533	1.00	24.87	N
ATOM	3399	CA	GLY	B	481	24.743	16.444	29.690	1.00	25.16	C
ATOM	3400	C	GLY	B	481	25.510	16.367	28.377	1.00	32.36	C
ATOM	3401	O	GLY	B	481	25.643	15.300	27.819	1.00	28.44	O
ATOM	3402	N	LEU	B	482	26.017	17.491	27.876	1.00	24.22	N
ATOM	3403	CA	LEU	B	482	26.778	17.474	26.617	1.00	24.32	C
ATOM	3404	CB	LEU	B	482	26.169	18.473	25.622	1.00	27.61	C
ATOM	3405	CG	LEU	B	482	24.767	18.111	25.133	1.00	31.09	C
ATOM	3406	CD1	LEU	B	482	24.143	19.316	24.392	1.00	37.33	C
ATOM	3407	CD2	LEU	B	482	24.868	16.912	24.231	1.00	33.44	C
ATOM	3408	C	LEU	B	482	28.229	17.843	26.833	1.00	20.28	C
ATOM	3409	O	LEU	B	482	28.998	18.006	25.881	1.00	27.53	O
ATOM	3410	N	SER	B	483	28.607	17.986	28.093	1.00	21.03	N
ATOM	3411	CA	SER	B	483	29.959	18.392	28.423	1.00	17.07	C
ATOM	3412	CB	SER	B	483	30.001	18.818	29.882	1.00	21.12	C
ATOM	3413	OG	SER	B	483	29.143	19.933	30.053	1.00	31.09	O
ATOM	3414	C	SER	B	483	30.984	17.298	28.156	1.00	21.12	C
ATOM	3415	O	SER	B	483	30.662	16.131	28.176	1.00	23.30	O
ATOM	3416	N	LYS	B	484	32.225	17.700	27.901	1.00	22.23	N
ATOM	3417	CA	LYS	B	484	33.281	16.732	27.641	1.00	22.46	C
ATOM	3418	CB	LYS	B	484	33.403	16.456	26.135	1.00	25.43	C
ATOM	3419	CG	LYS	B	484	32.202	15.661	25.564	1.00	37.37	C
ATOM	3420	CD	LYS	B	484	32.323	15.382	24.069	1.00	42.87	C
ATOM	3421	CE	LYS	B	484	31.228	14.402	23.622	1.00	42.01	C
ATOM	3422	NZ	LYS	B	484	29.878	14.732	24.149	1.00	57.01	N
ATOM	3423	C	LYS	B	484	34.622	17.227	28.157	1.00	26.66	C
ATOM	3424	O	LYS	B	484	34.870	18.426	28.229	1.00	25.66	O
ATOM	3425	N	ALA	B	485	35.489	16.280	28.492	1.00	22.91	N
ATOM	3426	CA	ALA	B	485	36.825	16.636	28.962	1.00	21.91	C
ATOM	3427	CB	ALA	B	485	37.359	15.560	29.932	1.00	32.95	C
ATOM	3428	C	ALA	B	485	37.689	16.684	27.679	1.00	29.52	C
ATOM	3429	O	ALA	B	485	37.552	15.827	26.804	1.00	32.44	O
ATOM	3430	N	LEU	B	486	38.546	17.694	27.576	1.00	24.43	N

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ATOM	3431	CA	LEU	B	486	39.419	17.841	26.403	1.00	19.74	C
ATOM	3432	CB	LEU	B	486	39.663	19.335	26.108	1.00	28.91	C
ATOM	3433	CG	LEU	B	486	38.582	20.155	25.390	1.00	28.77	C
ATOM	3434	CD1	LEU	B	486	38.967	21.633	25.336	1.00	34.39	C
ATOM	3435	CD2	LEU	B	486	38.408	19.629	24.006	1.00	36.84	C
ATOM	3436	C	LEU	B	486	40.794	17.187	26.636	1.00	31.66	C
ATOM	3437	O	LEU	B	486	41.477	16.831	25.690	1.00	34.07	O
ATOM	3438	N	GLY	B	487	41.203	17.066	27.897	1.00	30.25	N
ATOM	3439	CA	GLY	B	487	42.510	16.493	28.177	1.00	35.90	C
ATOM	3440	C	GLY	B	487	43.591	17.425	27.643	1.00	35.05	C
ATOM	3441	O	GLY	B	487	43.547	18.624	27.847	1.00	37.70	O
ATOM	3442	N	ALA	B	488	44.540	16.853	26.919	1.00	36.40	N
ATOM	3443	CA	ALA	B	488	45.644	17.630	26.364	1.00	41.44	C
ATOM	3444	CB	ALA	B	488	46.841	16.711	26.100	1.00	44.00	C
ATOM	3445	C	ALA	B	488	45.283	18.375	25.080	1.00	40.64	C
ATOM	3446	O	ALA	B	488	46.035	19.227	24.627	1.00	40.65	O
ATOM	3447	N	ASP	B	489	44.125	18.068	24.506	1.00	37.22	N
ATOM	3448	CA	ASP	B	489	43.706	18.723	23.255	1.00	35.43	C
ATOM	3449	CB	ASP	B	489	42.740	17.811	22.497	1.00	36.96	C
ATOM	3450	CG	ASP	B	489	43.331	16.450	22.240	1.00	48.65	C
ATOM	3451	OD1	ASP	B	489	44.563	16.383	22.017	1.00	51.66	O
ATOM	3452	OD2	ASP	B	489	42.571	15.457	22.249	1.00	47.30	O
ATOM	3453	C	ASP	B	489	43.062	20.090	23.440	1.00	31.19	C
ATOM	3454	O	ASP	B	489	42.545	20.391	24.502	1.00	31.54	O
ATOM	3455	N	ASP	B	490	43.085	20.911	22.387	1.00	28.93	N
ATOM	3456	CA	ASP	B	490	42.480	22.235	22.480	1.00	31.46	C
ATOM	3457	CB	ASP	B	490	43.333	23.272	21.742	1.00	36.63	C
ATOM	3458	CG	ASP	B	490	43.495	22.950	20.292	1.00	47.74	C
ATOM	3459	OD1	ASP	B	490	44.554	23.298	19.706	1.00	55.99	O
ATOM	3460	OD2	ASP	B	490	42.557	22.364	19.727	1.00	54.77	O
ATOM	3461	C	ASP	B	490	41.047	22.241	21.942	1.00	26.58	C
ATOM	3462	O	ASP	B	490	40.347	23.252	22.028	1.00	25.36	O
ATOM	3463	N	SER	B	491	40.599	21.115	21.398	1.00	24.18	N
ATOM	3464	CA	SER	B	491	39.215	21.008	20.901	1.00	21.95	C
ATOM	3465	CB	SER	B	491	39.067	21.782	19.592	1.00	33.37	C
ATOM	3466	OG	SER	B	491	39.830	21.147	18.559	1.00	33.09	O
ATOM	3467	C	SER	B	491	38.879	19.574	20.619	1.00	29.49	C
ATOM	3468	O	SER	B	491	39.754	18.698	20.726	1.00	26.31	O
ATOM	3469	N	TYR	B	492	37.611	19.310	20.296	1.00	23.30	N
ATOM	3470	CA	TYR	B	492	37.228	17.987	19.891	1.00	24.79	C
ATOM	3471	CB	TYR	B	492	36.708	17.112	21.060	1.00	24.52	C
ATOM	3472	CG	TYR	B	492	35.358	17.507	21.590	1.00	26.67	C
ATOM	3473	CD1	TYR	B	492	34.187	16.946	21.070	1.00	26.01	C
ATOM	3474	CE1	TYR	B	492	32.928	17.362	21.510	1.00	29.14	C
ATOM	3475	CD2	TYR	B	492	35.249	18.487	22.568	1.00	24.91	C
ATOM	3476	CE2	TYR	B	492	33.979	18.912	23.025	1.00	24.00	C
ATOM	3477	CZ	TYR	B	492	32.835	18.343	22.483	1.00	26.42	C
ATOM	3478	OH	TYR	B	492	31.589	18.775	22.887	1.00	26.61	O
ATOM	3479	C	TYR	B	492	36.180	18.166	18.803	1.00	20.40	C
ATOM	3480	O	TYR	B	492	35.632	19.255	18.622	1.00	22.94	O
ATOM	3481	N	TYR	B	493	35.960	17.099	18.050	1.00	20.88	N
ATOM	3482	CA	TYR	B	493	34.958	17.072	16.980	1.00	19.63	C
ATOM	3483	CB	TYR	B	493	35.559	16.596	15.671	1.00	21.26	C
ATOM	3484	CG	TYR	B	493	36.515	17.601	15.095	1.00	24.50	C
ATOM	3485	CD1	TYR	B	493	37.777	17.769	15.645	1.00	27.04	C
ATOM	3486	CE1	TYR	B	493	38.652	18.713	15.144	1.00	36.13	C
ATOM	3487	CD2	TYR	B	493	36.137	18.407	14.014	1.00	26.33	C
ATOM	3488	CE2	TYR	B	493	37.011	19.352	13.501	1.00	27.99	C
ATOM	3489	CZ	TYR	B	493	38.262	19.497	14.067	1.00	32.35	C
ATOM	3490	OH	TYR	B	493	39.144	20.396	13.526	1.00	33.44	O
ATOM	3491	C	TYR	B	493	33.944	16.069	17.468	1.00	21.80	C
ATOM	3492	O	TYR	B	493	34.293	14.925	17.800	1.00	22.36	O
ATOM	3493	N	THR	B	494	32.695	16.514	17.539	1.00	26.46	N
ATOM	3494	CA	THR	B	494	31.623	15.700	18.095	1.00	33.93	C
ATOM	3495	CB	THR	B	494	30.580	16.611	18.817	1.00	33.02	C
ATOM	3496	OG1	THR	B	494	29.647	15.794	19.538	1.00	40.25	O
ATOM	3497	CG2	THR	B	494	29.817	17.435	17.812	1.00	33.65	C
ATOM	3498	C	THR	B	494	30.875	14.851	17.104	1.00	36.70	C

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ATOM	3499	O	THR	B	494	30.757	15.179	15.921	1.00	28.58	O
ATOM	3500	N	ALA	B	495	30.294	13.773	17.611	1.00	44.45	N
ATOM	3501	CA	ALA	B	495	29.508	12.911	16.764	1.00	49.14	C
ATOM	3502	CB	ALA	B	495	29.442	11.529	17.370	1.00	47.66	C
ATOM	3503	C	ALA	B	495	28.108	13.503	16.624	1.00	49.65	C
ATOM	3504	O	ALA	B	495	27.651	14.233	17.498	1.00	48.99	O
ATOM	3505	N	ARG	B	496	27.446	13.194	15.519	1.00	53.97	N
ATOM	3506	CA	ARG	B	496	26.098	13.678	15.264	1.00	57.66	C
ATOM	3507	CB	ARG	B	496	25.804	13.674	13.759	1.00	60.80	C
ATOM	3508	CG	ARG	B	496	25.116	14.929	13.230	1.00	65.91	C
ATOM	3509	CD	ARG	B	496	23.905	15.299	14.043	1.00	66.81	C
ATOM	3510	NE	ARG	B	496	23.322	16.552	13.573	1.00	66.60	N
ATOM	3511	CZ	ARG	B	496	22.295	17.160	14.156	1.00	71.04	C
ATOM	3512	NH1	ARG	B	496	21.737	16.626	15.237	1.00	70.95	N
ATOM	3513	NH2	ARG	B	496	21.826	18.299	13.660	1.00	66.70	N
ATOM	3514	C	ARG	B	496	25.106	12.741	15.964	1.00	60.28	C
ATOM	3515	O	ARG	B	496	25.185	11.519	15.826	1.00	58.20	O
ATOM	3516	N	SER	B	497	24.183	13.316	16.721	1.00	58.58	N
ATOM	3517	CA	SER	B	497	23.175	12.513	17.407	1.00	60.66	C
ATOM	3518	CB	SER	B	497	23.267	12.711	18.920	1.00	58.31	C
ATOM	3519	OG	SER	B	497	22.882	14.026	19.276	1.00	66.25	O
ATOM	3520	C	SER	B	497	21.809	12.965	16.913	1.00	60.66	C
ATOM	3521	O	SER	B	497	21.711	13.896	16.114	1.00	59.92	O
ATOM	3522	N	ALA	B	498	20.764	12.305	17.396	1.00	63.28	N
ATOM	3523	CA	ALA	B	498	19.399	12.645	17.015	1.00	61.54	C
ATOM	3524	CB	ALA	B	498	18.440	11.531	17.450	1.00	58.15	C
ATOM	3525	C	ALA	B	498	18.995	13.963	17.671	1.00	60.15	C
ATOM	3526	O	ALA	B	498	19.422	14.275	18.783	1.00	59.70	O
ATOM	3527	N	GLY	B	499	18.168	14.733	16.977	1.00	61.09	N
ATOM	3528	CA	GLY	B	499	17.719	15.994	17.533	1.00	63.27	C
ATOM	3529	C	GLY	B	499	18.325	17.184	16.826	1.00	61.70	C
ATOM	3530	O	GLY	B	499	19.309	17.051	16.096	1.00	63.96	O
ATOM	3531	N	LYS	B	500	17.735	18.352	17.042	1.00	59.76	N
ATOM	3532	CA	LYS	B	500	18.216	19.576	16.417	1.00	57.53	C
ATOM	3533	CB	LYS	B	500	17.052	20.550	16.210	1.00	60.45	C
ATOM	3534	CG	LYS	B	500	16.017	20.091	15.199	1.00	61.48	C
ATOM	3535	CD	LYS	B	500	16.561	20.185	13.780	1.00	65.74	C
ATOM	3536	CE	LYS	B	500	15.500	19.800	12.756	1.00	62.41	C
ATOM	3537	NZ	LYS	B	500	16.013	19.898	11.358	1.00	67.47	N
ATOM	3538	C	LYS	B	500	19.283	20.251	17.275	1.00	51.49	C
ATOM	3539	O	LYS	B	500	19.282	20.137	18.495	1.00	49.86	O
ATOM	3540	N	TRP	B	501	20.195	20.957	16.618	1.00	45.23	N
ATOM	3541	CA	TRP	B	501	21.253	21.680	17.325	1.00	46.44	C
ATOM	3542	CB	TRP	B	501	22.530	21.673	16.483	1.00	40.73	C
ATOM	3543	CG	TRP	B	501	23.332	20.423	16.584	1.00	38.73	C
ATOM	3544	CD2	TRP	B	501	24.704	20.258	16.199	1.00	35.99	C
ATOM	3545	CE2	TRP	B	501	25.085	18.943	16.562	1.00	39.61	C
ATOM	3546	CE3	TRP	B	501	25.651	21.095	15.586	1.00	39.41	C
ATOM	3547	CD1	TRP	B	501	22.942	19.235	17.133	1.00	40.88	C
ATOM	3548	NE1	TRP	B	501	23.992	18.339	17.130	1.00	40.09	N
ATOM	3549	CZ2	TRP	B	501	26.375	18.448	16.337	1.00	35.77	C
ATOM	3550	CZ3	TRP	B	501	26.942	20.597	15.361	1.00	34.28	C
ATOM	3551	CH2	TRP	B	501	27.286	19.287	15.739	1.00	40.15	C
ATOM	3552	C	TRP	B	501	20.795	23.126	17.545	1.00	39.13	C
ATOM	3553	O	TRP	B	501	20.193	23.722	16.648	1.00	42.06	O
ATOM	3554	N	PRO	B	502	21.060	23.703	18.736	1.00	35.62	N
ATOM	3555	CD	PRO	B	502	21.732	23.060	19.884	1.00	36.26	C
ATOM	3556	CA	PRO	B	502	20.675	25.094	19.056	1.00	38.57	C
ATOM	3557	CB	PRO	B	502	20.841	25.158	20.569	1.00	36.44	C
ATOM	3558	CG	PRO	B	502	22.021	24.232	20.803	1.00	42.17	C
ATOM	3559	C	PRO	B	502	21.650	26.019	18.328	1.00	34.08	C
ATOM	3560	O	PRO	B	502	22.528	26.650	18.941	1.00	27.50	O
ATOM	3561	N	LEU	B	503	21.487	26.069	17.011	1.00	27.87	N
ATOM	3562	CA	LEU	B	503	22.377	26.847	16.147	1.00	30.99	C
ATOM	3563	CB	LEU	B	503	21.846	26.834	14.706	1.00	35.93	C
ATOM	3564	CG	LEU	B	503	21.555	25.457	14.117	1.00	38.86	C
ATOM	3565	CD1	LEU	B	503	20.943	25.607	12.720	1.00	46.43	C
ATOM	3566	CD2	LEU	B	503	22.833	24.656	14.046	1.00	42.19	C

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ATOM	3567	C	LEU	B	503	22.603	28.287	16.564	1.00	24.64	C
ATOM	3568	O	LEU	B	503	23.707	28.826	16.364	1.00	24.20	O
ATOM	3569	N	LYS	B	504	21.586	28.914	17.154	1.00	24.76	N
ATOM	3570	CA	LYS	B	504	21.712	30.313	17.542	1.00	26.03	C
ATOM	3571	CB	LYS	B	504	20.353	30.890	17.939	1.00	29.28	C
ATOM	3572	CG	LYS	B	504	19.400	31.000	16.729	1.00	31.16	C
ATOM	3573	CD	LYS	B	504	18.070	31.656	17.108	1.00	33.06	C
ATOM	3574	CE	LYS	B	504	17.121	31.755	15.913	1.00	34.32	C
ATOM	3575	NZ	LYS	B	504	15.941	32.606	16.264	1.00	37.82	N
ATOM	3576	C	LYS	B	504	22.726	30.552	18.657	1.00	28.80	C
ATOM	3577	O	LYS	B	504	23.130	31.663	18.884	1.00	20.01	O
ATOM	3578	N	TRP	B	505	23.141	29.497	19.338	1.00	23.22	N
ATOM	3579	CA	TRP	B	505	24.134	29.656	20.408	1.00	19.35	C
ATOM	3580	CB	TRP	B	505	23.681	28.883	21.665	1.00	25.81	C
ATOM	3581	CG	TRP	B	505	22.680	29.620	22.472	1.00	24.36	C
ATOM	3582	CD2	TRP	B	505	21.277	29.724	22.215	1.00	22.43	C
ATOM	3583	CE2	TRP	B	505	20.739	30.586	23.194	1.00	23.82	C
ATOM	3584	CE3	TRP	B	505	20.415	29.170	21.251	1.00	27.42	C
ATOM	3585	CD1	TRP	B	505	22.934	30.389	23.567	1.00	18.37	C
ATOM	3586	NE1	TRP	B	505	21.771	30.980	24.005	1.00	23.48	N
ATOM	3587	.CZ2	TRP	B	505	19.371	30.916	23.245	1.00	31.39	C
ATOM	3588	CZ3	TRP	B	505	19.051	29.496	21.299	1.00	28.93	C
ATOM	3589	CH2	TRP	B	505	18.547	30.365	22.296	1.00	25.25	C
ATOM	3590	C	TRP	B	505	25.497	29.098	19.954	1.00	19.69	C
ATOM	3591	O	TRP	B	505	26.496	29.233	20.663	1.00	22.22	O
ATOM	3592	N	TYR	B	506	25.546	28.513	18.767	1.00	21.76	N
ATOM	3593	CA	TYR	B	506	26.794	27.885	18.285	1.00	22.94	C
ATOM	3594	CB	TYR	B	506	26.426	26.615	17.488	1.00	21.82	C
ATOM	3595	CG	TYR	B	506	26.093	25.389	18.339	1.00	23.08	C
ATOM	3596	CD1	TYR	B	506	25.885	25.496	19.710	1.00	25.11	C
ATOM	3597	CE1	TYR	B	506	25.559	24.358	20.489	1.00	34.90	C
ATOM	3598	CD2	TYR	B	506	25.981	24.124	17.751	1.00	29.64	C
ATOM	3599	CE2	TYR	B	506	25.669	22.993	18.524	1.00	32.44	C
ATOM	3600	CZ	TYR	B	506	25.454	23.117	19.880	1.00	32.19	C
ATOM	3601	OH	TYR	B	506	25.086	22.008	20.619	1.00	37.37	O
ATOM	3602	C	TYR	B	506	27.745	28.757	17.434	1.00	28.60	C
ATOM	3603	O	TYR	B	506	27.299	29.447	16.524	1.00	25.58	O
ATOM	3604	N	ALA	B	507	29.048	28.703	17.731	1.00	23.48	N
ATOM	3605	CA	ALA	B	507	30.061	29.440	16.980	1.00	22.63	C
ATOM	3606	CB	ALA	B	507	31.443	29.298	17.674	1.00	19.24	C
ATOM	3607	C	ALA	B	507	30.122	28.845	15.567	1.00	24.54	C
ATOM	3608	O	ALA	B	507	29.709	27.709	15.343	1.00	23.92	O
ATOM	3609	N	PRO	B	508	30.659	29.597	14.603	1.00	22.52	N
ATOM	3610	CD	PRO	B	508	31.136	30.985	14.747	1.00	24.20	C
ATOM	3611	CA	PRO	B	508	30.772	29.135	13.212	1.00	23.99	C
ATOM	3612	CB	PRO	B	508	31.546	30.265	12.529	1.00	28.71	C
ATOM	3613	CG	PRO	B	508	31.113	31.477	13.328	1.00	35.43	C
ATOM	3614	C	PRO	B	508	31.452	27.787	13.007	1.00	23.80	C
ATOM	3615	O	PRO	B	508	30.960	26.964	12.231	1.00	23.69	O
ATOM	3616	N	GLU	B	509	32.576	27.568	13.695	1.00	22.83	N
ATOM	3617	CA	GLU	B	509	33.316	26.315	13.564	1.00	26.16	C
ATOM	3618	CB	GLU	B	509	34.689	26.390	14.268	1.00	26.11	C
ATOM	3619	CG	GLU	B	509	34.622	26.429	15.792	1.00	25.28	C
ATOM	3620	CD	GLU	B	509	34.538	27.843	16.341	1.00	30.45	C
ATOM	3621	OE1	GLU	B	509	34.270	28.798	15.561	1.00	24.15	O
ATOM	3622	OE2	GLU	B	509	34.716	27.989	17.568	1.00	25.31	O
ATOM	3623	C	GLU	B	509	32.512	25.128	14.098	1.00	22.82	C
ATOM	3624	O	GLU	B	509	32.751	23.992	13.686	1.00	25.61	O
ATOM	3625	N	CYS	B	510	31.571	25.389	15.010	1.00	20.67	N
ATOM	3626	CA	CYS	B	510	30.726	24.323	15.536	1.00	17.87	C
ATOM	3627	CB	CYS	B	510	29.867	24.838	16.704	1.00	17.65	C
ATOM	3628	SG	CYS	B	510	30.852	25.448	18.085	1.00	24.98	S
ATOM	3629	C	CYS	B	510	29.772	23.849	14.428	1.00	20.96	C
ATOM	3630	O	CYS	B	510	29.602	22.676	14.188	1.00	25.35	O
ATOM	3631	N	ILE	B	511	29.149	24.803	13.763	1.00	21.34	N
ATOM	3632	CA	ILE	B	511	28.188	24.473	12.713	1.00	26.63	C
ATOM	3633	CB	ILE	B	511	27.286	25.707	12.388	1.00	27.47	C
ATOM	3634	CG2	ILE	B	511	26.264	25.345	11.289	1.00	33.99	C

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ATOM	3635	CG1	ILE	B	511	26.574	26.153	13.671	1.00	26.92	C
ATOM	3636	CD1	ILE	B	511	25.895	27.516	13.597	1.00	31.85	C
ATOM	3637	C	ILE	B	511	28.871	23.984	11.446	1.00	30.34	C
ATOM	3638	O	ILE	B	511	28.434	22.987	10.848	1.00	29.71	O
ATOM	3639	N	ASN	B	512	29.968	24.623	11.058	1.00	25.07	N
ATOM	3640	CA	ASN	B	512	30.615	24.223	9.825	1.00	25.52	C
ATOM	3641	CB	ASN	B	512	31.416	25.376	9.236	1.00	23.08	C
ATOM	3642	CG	ASN	B	512	30.539	26.534	8.817	1.00	31.89	C
ATOM	3643	OD1	ASN	B	512	29.466	26.336	8.268	1.00	35.21	O
ATOM	3644	ND2	ASN	B	512	31.000	27.747	9.072	1.00	40.49	N
ATOM	3645	C	ASN	B	512	31.518	23.014	9.970	1.00	30.37	C
ATOM	3646	O	ASN	B	512	31.633	22.224	9.045	1.00	30.30	O
ATOM	3647	N	PHE	B	513	32.178	22.874	11.109	1.00	23.05	N
ATOM	3648	CA	PHE	B	513	33.084	21.744	11.273	1.00	21.06	C
ATOM	3649	CB	PHE	B	513	34.513	22.245	11.303	1.00	21.42	C
ATOM	3650	CG	PHE	B	513	34.924	22.945	10.031	1.00	32.74	C
ATOM	3651	CD1	PHE	B	513	35.063	24.326	10.005	1.00	34.47	C
ATOM	3652	CD2	PHE	B	513	35.120	22.216	8.858	1.00	32.93	C
ATOM	3653	CE1	PHE	B	513	35.393	24.986	8.805	1.00	39.39	C
ATOM	3654	CE2	PHE	B	513	35.448	22.871	7.664	1.00	40.01	C
ATOM	3655	CZ	PHE	B	513	35.581	24.253	7.645	1.00	36.34	C
ATOM	3656	C	PHE	B	513	32.856	20.836	12.477	1.00	24.61	C
ATOM	3657	O	PHE	B	513	33.687	19.968	12.741	1.00	25.10	O
ATOM	3658	N	ARG	B	514	31.758	21.060	13.207	1.00	20.51	N
ATOM	3659	CA	ARG	B	514	31.407	20.266	14.381	1.00	21.86	C
ATOM	3660	CB	ARG	B	514	31.062	18.815	13.944	1.00	21.50	C
ATOM	3661	CG	ARG	B	514	29.938	18.782	12.935	1.00	22.64	C
ATOM	3662	CD	ARG	B	514	29.437	17.415	12.570	1.00	25.89	C
ATOM	3663	NE	ARG	B	514	28.284	17.550	11.668	1.00	25.50	N
ATOM	3664	CZ	ARG	B	514	27.531	16.537	11.265	1.00	27.87	C
ATOM	3665	NH1	ARG	B	514	27.803	15.306	11.672	1.00	28.30	N
ATOM	3666	NH2	ARG	B	514	26.476	16.760	10.478	1.00	28.78	N
ATOM	3667	C	ARG	B	514	32.560	20.260	15.395	1.00	21.80	C
ATOM	3668	O	ARG	B	514	32.735	19.299	16.141	1.00	23.13	O
ATOM	3669	N	LYS	B	515	33.288	21.373	15.438	1.00	23.39	N
ATOM	3670	CA	LYS	B	515	34.442	21.512	16.323	1.00	21.15	C
ATOM	3671	CB	LYS	B	515	35.551	22.203	15.532	1.00	22.48	C
ATOM	3672	CG	LYS	B	515	36.848	22.399	16.309	1.00	23.37	C
ATOM	3673	CD	LYS	B	515	37.848	23.195	15.490	1.00	30.48	C
ATOM	3674	CE	LYS	B	515	38.992	23.662	16.372	1.00	37.06	C
ATOM	3675	NZ	LYS	B	515	39.892	24.621	15.659	1.00	43.43	N
ATOM	3676	C	LYS	B	515	34.100	22.315	17.597	1.00	22.11	C
ATOM	3677	O	LYS	B	515	33.704	23.477	17.503	1.00	20.32	O
ATOM	3678	N	PHE	B	516	34.302	21.712	18.773	1.00	22.31	N
ATOM	3679	CA	PHE	B	516	33.987	22.381	20.045	1.00	19.14	C
ATOM	3680	CB	PHE	B	516	32.903	21.592	20.788	1.00	20.60	C
ATOM	3681	CG	PHE	B	516	31.585	21.555	20.037	1.00	21.15	C
ATOM	3682	CD1	PHE	B	516	31.411	20.683	18.963	1.00	22.16	C
ATOM	3683	CD2	PHE	B	516	30.559	22.439	20.371	1.00	25.22	C
ATOM	3684	CE1	PHE	B	516	30.223	20.683	18.229	1.00	25.00	C
ATOM	3685	CE2	PHE	B	516	29.374	22.450	19.629	1.00	23.08	C
ATOM	3686	CZ	PHE	B	516	29.209	21.565	18.561	1.00	27.70	C
ATOM	3687	C	PHE	B	516	35.214	22.578	20.911	1.00	19.07	C
ATOM	3688	O	PHE	B	516	36.127	21.736	20.908	1.00	21.35	O
ATOM	3689	N	SER	B	517	35.206	23.667	21.684	1.00	19.27	N
ATOM	3690	CA	SER	B	517	36.366	24.059	22.496	1.00	26.23	C
ATOM	3691	CB	SER	B	517	37.385	24.718	21.542	1.00	24.44	C
ATOM	3692	OG	SER	B	517	36.770	25.861	20.910	1.00	22.44	O
ATOM	3693	C	SER	B	517	35.935	25.102	23.528	1.00	21.53	C
ATOM	3694	O	SER	B	517	34.792	25.509	23.523	1.00	20.37	O
ATOM	3695	N	SER	B	518	36.836	25.554	24.404	1.00	19.72	N
ATOM	3696	CA	SER	B	518	36.435	26.590	25.329	1.00	20.34	C
ATOM	3697	CB	SER	B	518	37.555	26.890	26.341	1.00	27.31	C
ATOM	3698	OG	SER	B	518	37.592	25.809	27.275	1.00	32.37	O
ATOM	3699	C	SER	B	518	36.039	27.842	24.551	1.00	21.23	C
ATOM	3700	O	SER	B	518	35.165	28.589	24.977	1.00	23.54	O
ATOM	3701	N	ARG	B	519	36.689	28.055	23.421	1.00	21.32	N
ATOM	3702	CA	ARG	B	519	36.347	29.205	22.610	1.00	18.97	C

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ATOM	3703	CB	ARG	B	519	37.414	29.420	21.545	1.00	21.22	C
ATOM	3704	CG	ARG	B	519	38.585	30.196	22.148	1.00	26.38	C
ATOM	3705	CD	ARG	B	519	39.753	30.191	21.208	1.00	35.68	C
ATOM	3706	NE	ARG	B	519	40.851	30.943	21.789	1.00	42.06	N
ATOM	3707	CZ	ARG	B	519	42.082	30.952	21.288	1.00	46.57	C
ATOM	3708	NH1	ARG	B	519	42.367	30.246	20.195	1.00	43.72	N
ATOM	3709	NH2	ARG	B	519	43.032	31.653	21.892	1.00	49.64	N
ATOM	3710	C	ARG	B	519	34.964	29.121	21.987	1.00	19.81	C
ATOM	3711	O	ARG	B	519	34.363	30.171	21.729	1.00	21.27	O
ATOM	3712	N	SER	B	520	34.460	27.909	21.718	1.00	18.58	N
ATOM	3713	CA	SER	B	520	33.075	27.864	21.213	1.00	21.84	C
ATOM	3714	CB	SER	B	520	32.742	26.535	20.503	1.00	20.81	C
ATOM	3715	OG	SER	B	520	32.908	25.379	21.297	1.00	22.92	O
ATOM	3716	C	SER	B	520	32.158	28.162	22.437	1.00	23.07	C
ATOM	3717	O	SER	B	520	31.091	28.760	22.290	1.00	21.17	O
ATOM	3718	N	ASP	B	521	32.597	27.810	23.649	1.00	19.80	N
ATOM	3719	CA	ASP	B	521	31.824	28.119	24.877	1.00	21.41	C
ATOM	3720	CB	ASP	B	521	32.462	27.523	26.150	1.00	28.78	C
ATOM	3721	CG	ASP	B	521	32.050	26.058	26.409	1.00	22.85	C
ATOM	3722	OD1	ASP	B	521	31.099	25.558	25.763	1.00	22.20	O
ATOM	3723	OD2	ASP	B	521	32.683	25.426	27.306	1.00	22.04	O
ATOM	3724	C	ASP	B	521	31.827	29.656	25.044	1.00	17.40	C
ATOM	3725	O	ASP	B	521	30.822	30.257	25.477	1.00	20.22	O
ATOM	3726	N	VAL	B	522	32.944	30.299	24.673	1.00	16.61	N
ATOM	3727	CA	VAL	B	522	32.990	31.785	24.758	1.00	15.75	C
ATOM	3728	CB	VAL	B	522	34.397	32.326	24.385	1.00	18.63	C
ATOM	3729	CG1	VAL	B	522	34.392	33.849	24.190	1.00	20.55	C
ATOM	3730	CG2	VAL	B	522	35.377	31.957	25.537	1.00	18.25	C
ATOM	3731	C	VAL	B	522	31.927	32.402	23.834	1.00	16.27	C
ATOM	3732	O	VAL	B	522	31.243	33.352	24.221	1.00	18.90	O
ATOM	3733	N	TRP	B	523	31.783	31.848	22.634	1.00	17.66	N
ATOM	3734	CA	TRP	B	523	30.758	32.371	21.708	1.00	16.82	C
ATOM	3735	CB	TRP	B	523	30.805	31.584	20.386	1.00	15.58	C
ATOM	3736	CG	TRP	B	523	29.813	32.106	19.335	1.00	17.41	C
ATOM	3737	CD2	TRP	B	523	30.129	32.847	18.145	1.00	19.38	C
ATOM	3738	CE2	TRP	B	523	28.904	33.164	17.516	1.00	20.03	C
ATOM	3739	CE3	TRP	B	523	31.332	33.280	17.546	1.00	18.44	C
ATOM	3740	CD1	TRP	B	523	28.448	31.999	19.375	1.00	22.97	C
ATOM	3741	NE1	TRP	B	523	27.891	32.641	18.280	1.00	18.65	N
ATOM	3742	CZ2	TRP	B	523	28.839	33.895	16.322	1.00	21.60	C
ATOM	3743	CZ3	TRP	B	523	31.263	34.010	16.359	1.00	19.75	C
ATOM	3744	CH2	TRP	B	523	30.030	34.313	15.758	1.00	19.91	C
ATOM	3745	C	TRP	B	523	29.373	32.241	22.358	1.00	18.12	C
ATOM	3746	O	TRP	B	523	28.573	33.189	22.321	1.00	19.38	O
ATOM	3747	N	SER	B	524	29.088	31.082	22.956	1.00	17.71	N
ATOM	3748	CA	SER	B	524	27.791	30.853	23.643	1.00	22.69	C
ATOM	3749	CB	SER	B	524	27.740	29.419	24.213	1.00	21.28	C
ATOM	3750	OG	SER	B	524	27.817	28.467	23.185	1.00	31.98	O
ATOM	3751	C	SER	B	524	27.579	31.829	24.792	1.00	22.41	C
ATOM	3752	O	SER	B	524	26.464	32.331	25.014	1.00	18.61	O
ATOM	3753	N	TYR	B	525	28.644	32.099	25.546	1.00	22.85	N
ATOM	3754	CA	TYR	B	525	28.619	33.051	26.640	1.00	21.01	C
ATOM	3755	CB	TYR	B	525	30.040	33.201	27.268	1.00	19.16	C
ATOM	3756	CG	TYR	B	525	30.046	34.181	28.409	1.00	20.09	C
ATOM	3757	CD1	TYR	B	525	29.456	33.865	29.638	1.00	21.83	C
ATOM	3758	CE1	TYR	B	525	29.411	34.806	30.692	1.00	20.51	C
ATOM	3759	CD2	TYR	B	525	30.602	35.461	28.251	1.00	19.44	C
ATOM	3760	CE2	TYR	B	525	30.553	36.400	29.286	1.00	21.12	C
ATOM	3761	CZ	TYR	B	525	29.956	36.066	30.501	1.00	26.32	C
ATOM	3762	OH	TYR	B	525	29.911	36.999	31.518	1.00	24.81	O
ATOM	3763	C	TYR	B	525	28.159	34.407	26.098	1.00	20.91	C
ATOM	3764	O	TYR	B	525	27.344	35.092	26.718	1.00	20.39	O
ATOM	3765	N	GLY	B	526	28.711	34.811	24.950	1.00	18.42	N
ATOM	3766	CA	GLY	B	526	28.306	36.086	24.357	1.00	19.09	C
ATOM	3767	C	GLY	B	526	26.803	36.116	24.081	1.00	16.71	C
ATOM	3768	O	GLY	B	526	26.135	37.118	24.371	1.00	19.95	O
ATOM	3769	N	VAL	B	527	26.271	35.039	23.506	1.00	19.63	N
ATOM	3770	CA	VAL	B	527	24.821	34.980	23.240	1.00	17.92	C

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ATOM	3771	CB	VAL	B	527	24.470	33.705	22.461	1.00	18.12	C
ATOM	3772	CG1	VAL	B	527	22.943	33.645	22.145	1.00	19.94	C
ATOM	3773	CG2	VAL	B	527	25.270	33.697	21.122	1.00	19.40	C
ATOM	3774	C	VAL	B	527	24.082	35.026	24.600	1.00	20.57	C
ATOM	3775	O	VAL	B	527	23.063	35.686	24.735	1.00	21.39	O
ATOM	3776	N	THR	B	528	24.633	34.377	25.619	1.00	20.54	N
ATOM	3777	CA	THR	B	528	24.010	34.397	26.949	1.00	18.80	C
ATOM	3778	CB	THR	B	528	24.768	33.458	27.906	1.00	20.59	C
ATOM	3779	OG1	THR	B	528	24.673	32.114	27.395	1.00	21.50	O
ATOM	3780	CG2	THR	B	528	24.169	33.499	29.287	1.00	22.95	C
ATOM	3781	C	THR	B	528	23.981	35.821	27.507	1.00	25.29	C
ATOM	3782	O	THR	B	528	22.972	36.235	28.084	1.00	19.03	O
ATOM	3783	N	MET	B	529	25.083	36.560	27.337	1.00	21.53	N
ATOM	3784	CA	MET	B	529	25.147	37.955	27.789	1.00	20.49	C
ATOM	3785	CB	MET	B	529	26.479	38.621	27.360	1.00	20.90	C
ATOM	3786	CG	MET	B	529	27.726	38.072	28.092	1.00	22.65	C
ATOM	3787	SD	MET	B	529	29.178	39.101	27.591	1.00	24.81	S
ATOM	3788	CE	MET	B	529	28.792	40.693	28.291	1.00	22.12	C
ATOM	3789	C	MET	B	529	24.013	38.740	27.103	1.00	19.53	C
ATOM	3790	O	MET	B	529	23.331	39.551	27.739	1.00	20.14	O
ATOM	3791	N	TRP	B	530	23.843	38.505	25.802	1.00	20.92	N
ATOM	3792	CA	TRP	B	530	22.800	39.234	25.035	1.00	19.60	C
ATOM	3793	CB	TRP	B	530	22.848	38.845	23.556	1.00	20.03	C
ATOM	3794	CG	TRP	B	530	21.996	39.725	22.693	1.00	18.41	C
ATOM	3795	CD2	TRP	B	530	20.610	39.533	22.395	1.00	19.07	C
ATOM	3796	CE2	TRP	B	530	20.191	40.635	21.590	1.00	20.94	C
ATOM	3797	CE3	TRP	B	530	19.678	38.543	22.726	1.00	22.34	C
ATOM	3798	CD1	TRP	B	530	22.373	40.909	22.072	1.00	18.66	C
ATOM	3799	NE1	TRP	B	530	21.276	41.460	21.399	1.00	21.22	N
ATOM	3800	CZ2	TRP	B	530	18.866	40.762	21.116	1.00	26.05	C
ATOM	3801	CZ3	TRP	B	530	18.369	38.673	22.254	1.00	23.03	C
ATOM	3802	CH2	TRP	B	530	17.978	39.770	21.462	1.00	27.41	C
ATOM	3803	C	TRP	B	530	21.403	38.947	25.567	1.00	21.14	C
ATOM	3804	O	TRP	B	530	20.607	39.880	25.807	1.00	22.19	O
ATOM	3805	N	GLU	B	531	21.101	37.665	25.754	1.00	21.34	N
ATOM	3806	CA	GLU	B	531	19.799	37.234	26.288	1.00	22.58	C
ATOM	3807	CB	GLU	B	531	19.785	35.725	26.566	1.00	23.47	C
ATOM	3808	CG	GLU	B	531	19.941	34.786	25.384	1.00	26.14	C
ATOM	3809	CD	GLU	B	531	19.873	33.318	25.844	1.00	26.77	C
ATOM	3810	OE1	GLU	B	531	20.953	32.715	26.078	1.00	22.88	O
ATOM	3811	OE2	GLU	B	531	18.731	32.788	25.983	1.00	27.11	O
ATOM	3812	C	GLU	B	531	19.548	37.897	27.617	1.00	20.02	C
ATOM	3813	O	GLU	B	531	18.432	38.384	27.895	1.00	23.77	O
ATOM	3814	N	ALA	B	532	20.565	37.903	28.478	1.00	20.17	N
ATOM	3815	CA	ALA	B	532	20.408	38.497	29.795	1.00	18.65	C
ATOM	3816	CB	ALA	B	532	21.617	38.155	30.711	1.00	20.90	C
ATOM	3817	C	ALA	B	532	20.204	39.994	29.776	1.00	24.11	C
ATOM	3818	O	ALA	B	532	19.290	40.506	30.425	1.00	20.67	O
ATOM	3819	N	LEU	B	533	21.062	40.701	29.045	1.00	24.27	N
ATOM	3820	CA	LEU	B	533	20.980	42.163	28.975	1.00	28.04	C
ATOM	3821	CB	LEU	B	533	22.282	42.737	28.376	1.00	22.81	C
ATOM	3822	CG	LEU	B	533	23.472	42.615	29.345	1.00	21.62	C
ATOM	3823	CD1	LEU	B	533	24.801	42.869	28.608	1.00	29.89	C
ATOM	3824	CD2	LEU	B	533	23.309	43.620	30.508	1.00	25.39	C
ATOM	3825	C	LEU	B	533	19.745	42.629	28.194	1.00	26.38	C
ATOM	3826	O	LEU	B	533	19.352	43.810	28.275	1.00	22.57	O
ATOM	3827	N	SER	B	534	19.122	41.702	27.464	1.00	21.44	N
ATOM	3828	CA	SER	B	534	17.888	41.991	26.714	1.00	23.07	C
ATOM	3829	CB	SER	B	534	17.862	41.187	25.429	1.00	21.95	C
ATOM	3830	OG	SER	B	534	18.842	41.679	24.534	1.00	31.02	O
ATOM	3831	C	SER	B	534	16.709	41.560	27.562	1.00	24.51	C
ATOM	3832	O	SER	B	534	15.571	41.538	27.106	1.00	27.12	O
ATOM	3833	N	TYR	B	535	17.000	41.199	28.803	1.00	25.92	N
ATOM	3834	CA	TYR	B	535	15.990	40.738	29.739	1.00	28.32	C
ATOM	3835	CB	TYR	B	535	15.102	41.910	30.198	1.00	28.47	C
ATOM	3836	CG	TYR	B	535	15.858	42.811	31.144	1.00	29.31	C
ATOM	3837	CD1	TYR	B	535	16.777	43.733	30.652	1.00	28.02	C
ATOM	3838	CE1	TYR	B	535	17.563	44.492	31.511	1.00	29.55	C

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ATOM	3839	CD2	TYR	B	535	15.736	42.679	32.526	1.00 28.97	C
ATOM	3840	CE2	TYR	B	535	16.514	43.434	33.395	1.00 30.17	C
ATOM	3841	CZ	TYR	B	535	17.431	44.341	32.874	1.00 22.54	C
ATOM	3842	OH	TYR	B	535	18.185	45.117	33.713	1.00 29.23	O
ATOM	3843	C	TYR	B	535	15.137	39.579	29.224	1.00 30.50	C
ATOM	3844	O	TYR	B	535	13.918	39.637	29.245	1.00 29.15	O
ATOM	3845	N	GLY	B	536	15.805	38.525	28.754	1.00 25.34	N
ATOM	3846	CA	GLY	B	536	15.090	37.334	28.313	1.00 26.66	C
ATOM	3847	C	GLY	B	536	14.563	37.236	26.907	1.00 28.90	C
ATOM	3848	O	GLY	B	536	13.831	36.301	26.583	1.00 34.84	O
ATOM	3849	N	GLN	B	537	14.940	38.177	26.044	1.00 30.40	N
ATOM	3850	CA	GLN	B	537	14.504	38.138	24.658	1.00 28.41	C
ATOM	3851	CB	GLN	B	537	14.840	39.463	23.973	1.00 32.82	C
ATOM	3852	CG	GLN	B	537	13.837	40.571	24.309	1.00 43.11	C
ATOM	3853	CD	GLN	B	537	14.217	41.920	23.731	1.00 47.65	C
ATOM	3854	OE1	GLN	B	537	14.599	42.029	22.562	1.00 54.72	O
ATOM	3855	NE2	GLN	B	537	14.108	42.961	24.547	1.00 50.31	N
ATOM	3856	C	GLN	B	537	15.175	36.979	23.918	1.00 30.53	C
ATOM	3857	O	GLN	B	537	16.238	36.507	24.326	1.00 25.81	O
ATOM	3858	N	LYS	B	538	14.550	36.515	22.832	1.00 26.52	N
ATOM	3859	CA	LYS	B	538	15.124	35.429	22.060	1.00 26.82	C
ATOM	3860	CB	LYS	B	538	14.036	34.673	21.292	1.00 33.23	C
ATOM	3861	CG	LYS	B	538	13.077	33.922	22.201	1.00 43.54	C
ATOM	3862	CD	LYS	B	538	12.031	33.160	21.393	1.00 44.85	C
ATOM	3863	CE	LYS	B	538	11.278	32.173	22.282	1.00 50.77	C
ATOM	3864	NZ	LYS	B	538	10.275	31.376	21.506	1.00 55.00	N
ATOM	3865	C	LYS	B	538	16.142	35.971	21.055	1.00 28.86	C
ATOM	3866	O	LYS	B	538	15.915	37.005	20.425	1.00 29.11	O
ATOM	3867	N	PRO	B	539	17.289	35.290	20.917	1.00 25.45	N
ATOM	3868	CD	PRO	B	539	17.826	34.185	21.727	1.00 22.65	C
ATOM	3869	CA	PRO	B	539	18.285	35.763	19.952	1.00 24.40	C
ATOM	3870	CB	PRO	B	539	19.518	34.912	20.276	1.00 28.27	C
ATOM	3871	CG	PRO	B	539	18.920	33.647	20.824	1.00 33.25	C
ATOM	3872	C	PRO	B	539	17.828	35.548	18.507	1.00 28.17	C
ATOM	3873	O	PRO	B	539	17.136	34.582	18.201	1.00 25.84	O
ATOM	3874	N	TYR	B	540	18.229	36.458	17.630	1.00 22.91	N
ATOM	3875	CA	TYR	B	540	17.918	36.423	16.206	1.00 26.70	C
ATOM	3876	CB	TYR	B	540	18.740	35.333	15.518	1.00 23.59	C
ATOM	3877	CG	TYR	B	540	20.240	35.373	15.839	1.00 29.92	C
ATOM	3878	CD1	TYR	B	540	21.094	36.237	15.163	1.00 24.88	C
ATOM	3879	CE1	TYR	B	540	22.470	36.264	15.447	1.00 24.04	C
ATOM	3880	CD2	TYR	B	540	20.773	34.542	16.821	1.00 28.81	C
ATOM	3881	CE2	TYR	B	540	22.153	34.568	17.142	1.00 22.99	C
ATOM	3882	CZ	TYR	B	540	22.988	35.424	16.443	1.00 20.60	C
ATOM	3883	OH	TYR	B	540	24.327	35.447	16.724	1.00 23.56	O
ATOM	3884	C	TYR	B	540	16.435	36.134	16.017	1.00 25.23	C
ATOM	3885	O	TYR	B	540	16.063	35.273	15.224	1.00 28.39	O
ATOM	3886	N	LYS	B	541	15.637	36.889	16.769	1.00 28.66	N
ATOM	3887	CA	LYS	B	541	14.186	36.785	16.823	1.00 40.37	C
ATOM	3888	CB	LYS	B	541	13.642	38.072	17.450	1.00 43.79	C
ATOM	3889	CG	LYS	B	541	12.245	37.962	18.030	1.00 55.46	C
ATOM	3890	CD	LYS	B	541	11.876	39.211	18.856	1.00 55.84	C
ATOM	3891	CE	LYS	B	541	12.786	39.383	20.081	1.00 60.14	C
ATOM	3892	NZ	LYS	B	541	12.345	40.490	20.993	1.00 56.25	N
ATOM	3893	C	LYS	B	541	13.502	36.524	15.480	1.00 43.30	C
ATOM	3894	O	LYS	B	541	12.731	35.578	15.337	1.00 43.84	O
ATOM	3895	N	LYS	B	542	13.791	37.349	14.493	1.00 43.89	N
ATOM	3896	CA	LYS	B	542	13.147	37.178	13.200	1.00 50.62	C
ATOM	3897	CB	LYS	B	542	12.893	38.547	12.575	1.00 51.21	C
ATOM	3898	CG	LYS	B	542	14.153	39.355	12.339	1.00 56.73	C
ATOM	3899	CD	LYS	B	542	13.849	40.636	11.571	1.00 61.48	C
ATOM	3900	CE	LYS	B	542	15.135	41.350	11.161	1.00 60.94	C
ATOM	3901	NZ	LYS	B	542	14.892	42.611	10.395	1.00 64.23	N
ATOM	3902	C	LYS	B	542	13.921	36.309	12.221	1.00 56.90	C
ATOM	3903	O	LYS	B	542	13.821	36.518	11.008	1.00 59.68	O
ATOM	3904	N	MET	B	543	14.663	35.322	12.724	1.00 41.97	N
ATOM	3905	CA	MET	B	543	15.443	34.453	11.844	1.00 45.64	C
ATOM	3906	CB	MET	B	543	16.925	34.817	11.907	1.00 43.71	C

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ATOM	3907	CG	MET	B	543	17.348	35.994	11.066	1.00	53.65	C
ATOM	3908	SD	MET	B	543	19.100	36.330	11.367	1.00	42.99	S
ATOM	3909	CE	MET	B	543	18.961	37.898	12.209	1.00	45.52	C
ATOM	3910	C	MET	B	543	15.332	32.979	12.173	1.00	47.61	C
ATOM	3911	O	MET	B	543	15.075	32.599	13.318	1.00	48.77	O
ATOM	3912	N	LYS	B	544	15.562	32.152	11.157	1.00	48.07	N
ATOM	3913	CA	LYS	B	544	15.522	30.704	11.301	1.00	54.78	C
ATOM	3914	CB	LYS	B	544	14.693	30.079	10.181	1.00	55.48	C
ATOM	3915	CG	LYS	B	544	15.303	30.244	8.792	1.00	64.05	C
ATOM	3916	CD	LYS	B	544	14.493	29.491	7.739	1.00	64.50	C
ATOM	3917	CE	LYS	B	544	15.167	29.517	6.367	1.00	65.75	C
ATOM	3918	NZ	LYS	B	544	14.420	28.692	5.363	1.00	63.25	N
ATOM	3919	C	LYS	B	544	16.953	30.168	11.231	1.00	56.68	C
ATOM	3920	O	LYS	B	544	17.908	30.904	11.473	1.00	54.87	O
ATOM	3921	N	GLY	B	545	17.092	28.890	10.885	1.00	54.19	N
ATOM	3922	CA	GLY	B	545	18.408	28.280	10.805	1.00	51.15	C
ATOM	3923	C	GLY	B	545	19.352	28.912	9.797	1.00	50.65	C
ATOM	3924	O	GLY	B	545	20.219	29.694	10.174	1.00	52.75	O
ATOM	3925	N	PRO	B	546	19.213	28.585	8.504	1.00	50.84	N
ATOM	3926	CD	PRO	B	546	18.223	27.634	7.965	1.00	54.61	C
ATOM	3927	CA	PRO	B	546	20.056	29.110	7.423	1.00	51.43	C
ATOM	3928	CB	PRO	B	546	19.341	28.613	6.164	1.00	52.58	C
ATOM	3929	CG	PRO	B	546	18.809	27.294	6.609	1.00	51.61	C
ATOM	3930	C	PRO	B	546	20.241	30.624	7.416	1.00	45.67	C
ATOM	3931	O	PRO	B	546	21.274	31.128	6.963	1.00	40.66	O
ATOM	3932	N	GLU	B	547	19.234	31.343	7.903	1.00	40.50	N
ATOM	3933	CA	GLU	B	547	19.294	32.796	7.953	1.00	44.42	C
ATOM	3934	CB	GLU	B	547	17.963	33.376	8.410	1.00	44.41	C
ATOM	3935	CG	GLU	B	547	16.811	33.093	7.475	1.00	59.26	C
ATOM	3936	CD	GLU	B	547	15.538	33.763	7.927	1.00	56.22	C
ATOM	3937	OE1	GLU	B	547	15.479	35.013	7.898	1.00	62.09	O
ATOM	3938	OE2	GLU	B	547	14.603	33.037	8.319	1.00	59.62	O
ATOM	3939	C	GLU	B	547	20.391	33.282	8.902	1.00	35.91	C
ATOM	3940	O	GLU	B	547	21.149	34.172	8.555	1.00	34.83	O
ATOM	3941	N	VAL	B	548	20.460	32.694	10.094	1.00	36.33	N
ATOM	3942	CA	VAL	B	548	21.473	33.108	11.080	1.00	26.71	C
ATOM	3943	CB	VAL	B	548	21.252	32.396	12.420	1.00	35.48	C
ATOM	3944	CG1	VAL	B	548	22.285	32.872	13.448	1.00	32.82	C
ATOM	3945	CG2	VAL	B	548	19.847	32.688	12.917	1.00	40.22	C
ATOM	3946	C	VAL	B	548	22.890	32.843	10.591	1.00	31.26	C
ATOM	3947	O	VAL	B	548	23.762	33.696	10.708	1.00	33.92	O
ATOM	3948	N	MET	B	549	23.125	31.663	10.027	1.00	31.21	N
ATOM	3949	CA	MET	B	549	24.439	31.316	9.511	1.00	35.46	C
ATOM	3950	CB	MET	B	549	24.397	29.909	8.908	1.00	40.89	C
ATOM	3951	CG	MET	B	549	25.766	29.271	8.799	1.00	51.71	C
ATOM	3952	SD	MET	B	549	26.636	29.238	10.404	1.00	72.82	S
ATOM	3953	CE	MET	B	549	27.806	30.616	10.266	1.00	56.71	C
ATOM	3954	C	MET	B	549	24.918	32.325	8.445	1.00	31.51	C
ATOM	3955	O	MET	B	549	26.050	32.788	8.479	1.00	31.13	O
ATOM	3956	N	ALA	B	550	24.042	32.645	7.501	1.00	32.16	N
ATOM	3957	CA	ALA	B	550	24.373	33.588	6.431	1.00	33.32	C
ATOM	3958	CB	ALA	B	550	23.206	33.653	5.428	1.00	37.58	C
ATOM	3959	C	ALA	B	550	24.656	34.979	7.014	1.00	25.47	C
ATOM	3960	O	ALA	B	550	25.568	35.680	6.578	1.00	29.24	O
ATOM	3961	N	PHE	B	551	23.857	35.360	8.007	1.00	25.23	N
ATOM	3962	CA	PHE	B	551	23.975	36.647	8.706	1.00	28.55	C
ATOM	3963	CB	PHE	B	551	22.852	36.714	9.769	1.00	20.31	C
ATOM	3964	CG	PHE	B	551	22.783	38.000	10.543	1.00	29.64	C
ATOM	3965	CD1	PHE	B	551	22.226	39.144	9.973	1.00	28.55	C
ATOM	3966	CD2	PHE	B	551	23.209	38.052	11.876	1.00	29.88	C
ATOM	3967	CE1	PHE	B	551	22.081	40.319	10.716	1.00	26.70	C
ATOM	3968	CE2	PHE	B	551	23.066	39.232	12.636	1.00	26.29	C
ATOM	3969	CZ	PHE	B	551	22.498	40.362	12.050	1.00	31.05	C
ATOM	3970	C	PHE	B	551	25.354	36.743	9.361	1.00	26.40	C
ATOM	3971	O	PHE	B	551	26.084	37.721	9.188	1.00	22.68	O
ATOM	3972	N	ILE	B	552	25.717	35.720	10.123	1.00	23.43	N
ATOM	3973	CA	ILE	B	552	27.022	35.707	10.778	1.00	21.41	C
ATOM	3974	CB	ILE	B	552	27.135	34.460	11.681	1.00	26.93	C

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ATOM	3975	CG2	ILE	B	552	28.553	34.320	12.206	1.00	28.00	C
ATOM	3976	CG1	ILE	B	552	26.046	34.533	12.764	1.00	27.40	C
ATOM	3977	CD1	ILE	B	552	26.179	35.709	13.768	1.00	29.73	C
ATOM	3978	C	ILE	B	552	28.146	35.706	9.737	1.00	22.04	C
ATOM	3979	O	ILE	B	552	29.139	36.428	9.871	1.00	25.44	O
ATOM	3980	N	GLU	B	553	27.988	34.910	8.684	1.00	25.85	N
ATOM	3981	CA	GLU	B	553	29.004	34.842	7.630	1.00	30.95	C
ATOM	3982	CB	GLU	B	553	28.613	33.796	6.580	1.00	40.19	C
ATOM	3983	CG	GLU	B	553	28.654	32.360	7.092	1.00	48.42	C
ATOM	3984	CD	GLU	B	553	30.068	31.858	7.339	1.00	49.16	C
ATOM	3985	OE1	GLU	B	553	30.212	30.786	7.970	1.00	54.92	O
ATOM	3986	OE2	GLU	B	553	31.030	32.525	6.896	1.00	56.67	O
ATOM	3987	C	GLU	B	553	29.220	36.206	6.947	1.00	29.01	C
ATOM	3988	O	GLU	B	553	30.331	36.527	6.525	1.00	34.32	O
ATOM	3989	N	GLN	B	554	28.152	36.988	6.835	1.00	30.24	N
ATOM	3990	CA	GLN	B	554	28.214	38.324	6.240	1.00	33.67	C
ATOM	3991	CB	GLN	B	554	26.806	38.870	6.010	1.00	35.02	C
ATOM	3992	CG	GLN	B	554	26.026	38.224	4.891	1.00	47.06	C
ATOM	3993	CD	GLN	B	554	24.620	38.761	4.858	1.00	45.80	C
ATOM	3994	OE1	GLN	B	554	24.410	39.970	5.004	1.00	52.95	O
ATOM	3995	NE2	GLN	B	554	23.647	37.874	4.669	1.00	52.85	N
ATOM	3996	C	GLN	B	554	28.940	39.308	7.154	1.00	35.79	C
ATOM	3997	O	GLN	B	554	29.176	40.452	6.772	1.00	29.12	O
ATOM	3998	N	GLY	B	555	29.274	38.871	8.366	1.00	26.81	N
ATOM	3999	CA	GLY	B	555	29.960	39.765	9.284	1.00	29.43	C
ATOM	4000	C	GLY	B	555	29.025	40.644	10.119	1.00	27.00	C
ATOM	4001	O	GLY	B	555	29.447	41.672	10.660	1.00	26.99	O
ATOM	4002	N	LYS	B	556	27.759	40.257	10.231	1.00	20.65	N
ATOM	4003	CA	LYS	B	556	26.826	41.024	11.045	1.00	21.47	C
ATOM	4004	CB	LYS	B	556	25.489	41.198	10.315	1.00	24.59	C
ATOM	4005	CG	LYS	B	556	25.631	41.916	8.959	1.00	24.98	C
ATOM	4006	CD	LYS	B	556	24.280	42.165	8.338	1.00	24.97	C
ATOM	4007	CE	LYS	B	556	24.429	42.911	6.990	1.00	31.95	C
ATOM	4008	NZ	LYS	B	556	23.084	43.238	6.391	1.00	32.23	N
ATOM	4009	C	LYS	B	556	26.580	40.283	12.364	1.00	22.25	C
ATOM	4010	O	LYS	B	556	26.701	39.057	12.431	1.00	21.17	O
ATOM	4011	N	ARG	B	557	26.208	41.049	13.384	1.00	20.82	N
ATOM	4012	CA	ARG	B	557	25.950	40.496	14.709	1.00	22.17	C
ATOM	4013	CB	ARG	B	557	27.164	40.778	15.629	1.00	19.79	C
ATOM	4014	CG	ARG	B	557	28.487	40.159	15.124	1.00	21.41	C
ATOM	4015	CD	ARG	B	557	28.495	38.618	15.195	1.00	19.59	C
ATOM	4016	NE	ARG	B	557	29.796	38.029	14.814	1.00	20.25	N
ATOM	4017	CZ	ARG	B	557	30.161	37.681	13.579	1.00	23.23	C
ATOM	4018	NH1	ARG	B	557	29.329	37.849	12.534	1.00	21.34	N
ATOM	4019	NH2	ARG	B	557	31.354	37.117	13.379	1.00	18.85	N
ATOM	4020	C	ARG	B	557	24.699	41.113	15.311	1.00	25.58	C
ATOM	4021	O	ARG	B	557	24.163	42.122	14.787	1.00	20.60	O
ATOM	4022	N	MET	B	558	24.211	40.520	16.405	1.00	23.12	N
ATOM	4023	CA	MET	B	558	23.031	41.057	17.061	1.00	23.08	C
ATOM	4024	CB	MET	B	558	22.577	40.150	18.226	1.00	21.21	C
ATOM	4025	CG	MET	B	558	21.929	38.861	17.759	1.00	23.06	C
ATOM	4026	SD	MET	B	558	21.172	37.972	19.155	1.00	25.40	S
ATOM	4027	CE	MET	B	558	22.589	37.274	19.959	1.00	20.17	C
ATOM	4028	C	MET	B	558	23.299	42.458	17.588	1.00	26.20	C
ATOM	4029	O	MET	B	558	24.416	42.787	18.026	1.00	22.21	O
ATOM	4030	N	GLU	B	559	22.262	43.287	17.554	1.00	22.33	N
ATOM	4031	CA	GLU	B	559	22.354	44.649	18.023	1.00	25.04	C
ATOM	4032	CB	GLU	B	559	21.047	45.392	17.711	1.00	33.85	C
ATOM	4033	CG	GLU	B	559	19.765	44.572	17.953	1.00	44.82	C
ATOM	4034	CD	GLU	B	559	19.514	43.500	16.868	1.00	56.27	C
ATOM	4035	OE1	GLU	B	559	19.120	43.868	15.733	1.00	60.02	O
ATOM	4036	OE2	GLU	B	559	19.710	42.290	17.149	1.00	44.19	O
ATOM	4037	C	GLU	B	559	22.646	44.778	19.513	1.00	25.59	C
ATOM	4038	O	GLU	B	559	22.362	43.880	20.302	1.00	29.33	O
ATOM	4039	N	CYS	B	560	23.210	45.913	19.897	1.00	22.19	N
ATOM	4040	CA	CYS	B	560	23.471	46.170	21.306	1.00	25.34	C
ATOM	4041	CB	CYS	B	560	24.313	47.440	21.454	1.00	26.43	C
ATOM	4042	SG	CYS	B	560	24.611	47.893	23.164	1.00	30.43	S

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ATOM	4043	C	CYS	B	560	22.108	46.336	22.013	1.00	32.06	C
ATOM	4044	O	CYS	B	560	21.262	47.124	21.570	1.00	29.35	O
ATOM	4045	N	PRO	B	561	21.855	45.564	23.092	1.00	30.63	N
ATOM	4046	CD	PRO	B	561	22.644	44.426	23.611	1.00	28.65	C
ATOM	4047	CA	PRO	B	561	20.570	45.686	23.803	1.00	31.69	C
ATOM	4048	CB	PRO	B	561	20.727	44.723	24.987	1.00	28.11	C
ATOM	4049	CG	PRO	B	561	21.605	43.638	24.418	1.00	25.66	C
ATOM	4050	C	PRO	B	561	20.348	47.111	24.298	1.00	28.57	C
ATOM	4051	O	PRO	B	561	21.292	47.850	24.542	1.00	26.62	O
ATOM	4052	N	PRO	B	562	19.092	47.519	24.459	1.00	37.07	N
ATOM	4053	CD	PRO	B	562	17.852	46.840	24.046	1.00	39.32	C
ATOM	4054	CA	PRO	B	562	18.821	48.880	24.939	1.00	38.49	C
ATOM	4055	CB	PRO	B	562	17.294	48.942	24.948	1.00	42.66	C
ATOM	4056	CG	PRO	B	562	16.920	48.002	23.833	1.00	48.28	C
ATOM	4057	C	PRO	B	562	19.419	49.086	26.336	1.00	38.16	C
ATOM	4058	O	PRO	B	562	19.329	48.207	27.193	1.00	38.50	O
ATOM	4059	N	GLU	B	563	20.042	50.236	26.568	1.00	37.38	N
ATOM	4060	CA	GLU	B	563	20.623	50.530	27.881	1.00	43.37	C
ATOM	4061	CB	GLU	B	563	19.564	50.341	28.981	1.00	49.78	C
ATOM	4062	CG	GLU	B	563	18.309	51.190	28.805	1.00	53.84	C
ATOM	4063	CD	GLU	B	563	17.088	50.587	29.496	1.00	61.69	C
ATOM	4064	OE1	GLU	B	563	17.133	50.389	30.734	1.00	64.80	O
ATOM	4065	OE2	GLU	B	563	16.085	50.307	28.795	1.00	62.44	O
ATOM	4066	C	GLU	B	563	21.873	49.714	28.228	1.00	42.92	C
ATOM	4067	O	GLU	B	563	22.433	49.860	29.314	1.00	46.04	O
ATOM	4068	N	CYS	B	564	22.312	48.832	27.332	1.00	40.16	N
ATOM	4069	CA	CYS	B	564	23.527	48.070	27.589	1.00	35.91	C
ATOM	4070	CB	CYS	B	564	23.614	46.843	26.662	1.00	35.94	C
ATOM	4071	SG	CYS	B	564	25.157	45.907	26.802	1.00	37.39	S
ATOM	4072	C	CYS	B	564	24.706	49.006	27.324	1.00	37.21	C
ATOM	4073	O	CYS	B	564	24.832	49.559	26.231	1.00	36.78	O
ATOM	4074	N	PRO	B	565	25.580	49.200	28.324	1.00	35.01	N
ATOM	4075	CD	PRO	B	565	25.531	48.573	29.655	1.00	39.96	C
ATOM	4076	CA	PRO	B	565	26.753	50.072	28.200	1.00	32.47	C
ATOM	4077	CB	PRO	B	565	27.382	50.015	29.589	1.00	40.02	C
ATOM	4078	CG	PRO	B	565	26.960	48.666	30.098	1.00	43.81	C
ATOM	4079	C	PRO	B	565	27.709	49.607	27.127	1.00	35.02	C
ATOM	4080	O	PRO	B	565	27.860	48.403	26.893	1.00	34.15	O
ATOM	4081	N	PRO	B	566	28.396	50.558	26.475	1.00	33.68	N
ATOM	4082	CD	PRO	B	566	28.297	52.010	26.727	1.00	34.27	C
ATOM	4083	CA	PRO	B	566	29.360	50.272	25.408	1.00	30.53	C
ATOM	4084	CB	PRO	B	566	29.998	51.647	25.137	1.00	31.64	C
ATOM	4085	CG	PRO	B	566	28.908	52.607	25.481	1.00	31.51	C
ATOM	4086	C	PRO	B	566	30.412	49.223	25.792	1.00	31.72	C
ATOM	4087	O	PRO	B	566	30.757	48.379	24.978	1.00	28.48	O
ATOM	4088	N	GLU	B	567	30.920	49.285	27.028	1.00	27.33	N
ATOM	4089	CA	GLU	B	567	31.960	48.345	27.472	1.00	33.27	C
ATOM	4090	CB	GLU	B	567	32.451	48.701	28.894	1.00	36.30	C
ATOM	4091	CG	GLU	B	567	32.553	50.189	29.192	1.00	49.34	C
ATOM	4092	CD	GLU	B	567	31.195	50.835	29.391	1.00	50.90	C
ATOM	4093	OE1	GLU	B	567	30.471	50.431	30.330	1.00	63.92	O
ATOM	4094	OE2	GLU	B	567	30.851	51.744	28.612	1.00	47.96	O
ATOM	4095	C	GLU	B	567	31.440	46.908	27.485	1.00	26.60	C
ATOM	4096	O	GLU	B	567	32.143	45.964	27.089	1.00	25.31	O
ATOM	4097	N	LEU	B	568	30.208	46.747	27.948	1.00	25.52	N
ATOM	4098	CA	LEU	B	568	29.590	45.442	28.017	1.00	28.35	C
ATOM	4099	CB	LEU	B	568	28.312	45.549	28.851	1.00	31.11	C
ATOM	4100	CG	LEU	B	568	27.993	44.399	29.788	1.00	31.00	C
ATOM	4101	CD1	LEU	B	568	29.277	43.796	30.349	1.00	35.96	C
ATOM	4102	CD2	LEU	B	568	27.101	44.939	30.912	1.00	25.70	C
ATOM	4103	C	LEU	B	568	29.289	44.925	26.621	1.00	30.51	C
ATOM	4104	O	LEU	B	568	29.498	43.738	26.341	1.00	22.86	O
ATOM	4105	N	TYR	B	569	28.793	45.791	25.733	1.00	23.22	N
ATOM	4106	CA	TYR	B	569	28.538	45.310	24.383	1.00	22.95	C
ATOM	4107	CB	TYR	B	569	27.765	46.361	23.542	1.00	21.93	C
ATOM	4108	CG	TYR	B	569	27.412	45.828	22.170	1.00	21.83	C
ATOM	4109	CD1	TYR	B	569	26.583	44.721	22.022	1.00	21.17	C
ATOM	4110	CE1	TYR	B	569	26.304	44.169	20.757	1.00	22.67	C

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ATOM	4111	CD2	TYR	B	569	27.966	46.396	21.006	1.00 28.53	C
ATOM	4112	CE2	TYR	B	569	27.703	45.853	19.739	1.00 27.28	C
ATOM	4113	CZ	TYR	B	569	26.881	44.746	19.622	1.00 28.33	C
ATOM	4114	OH	TYR	B	569	26.664	44.202	18.384	1.00 25.54	O
ATOM	4115	C	TYR	B	569	29.856	44.948	23.683	1.00 19.58	C
ATOM	4116	O	TYR	B	569	29.909	43.976	22.908	1.00 23.18	O
ATOM	4117	N	ALA	B	570	30.927	45.704	23.943	1.00 23.62	N
ATOM	4118	CA	ALA	B	570	32.206	45.415	23.296	1.00 24.27	C
ATOM	4119	CB	ALA	B	570	33.287	46.413	23.739	1.00 26.06	C
ATOM	4120	C	ALA	B	570	32.670	43.993	23.615	1.00 24.88	C
ATOM	4121	O	ALA	B	570	33.226	43.307	22.768	1.00 23.64	O
ATOM	4122	N	LEU	B	571	32.443	43.587	24.856	1.00 23.04	N
ATOM	4123	CA	LEU	B	571	32.844	42.259	25.336	1.00 21.51	C
ATOM	4124	CB	LEU	B	571	32.668	42.201	26.866	1.00 23.34	C
ATOM	4125	CG	LEU	B	571	32.928	40.815	27.465	1.00 22.60	C
ATOM	4126	CD1	LEU	B	571	34.295	40.301	27.028	1.00 24.30	C
ATOM	4127	CD2	LEU	B	571	32.820	40.914	28.981	1.00 24.39	C
ATOM	4128	C	LEU	B	571	31.988	41.197	24.676	1.00 16.75	C
ATOM	4129	O	LEU	B	571	32.472	40.189	24.163	1.00 20.66	O
ATOM	4130	N	MET	B	572	30.687	41.427	24.715	1.00 20.93	N
ATOM	4131	CA	MET	B	572	29.728	40.535	24.102	1.00 20.96	C
ATOM	4132	CB	MET	B	572	28.356	41.204	24.223	1.00 28.64	C
ATOM	4133	CG	MET	B	572	27.271	40.510	23.502	1.00 30.16	C
ATOM	4134	SD	MET	B	572	25.729	41.414	23.691	1.00 24.19	S
ATOM	4135	CE	MET	B	572	25.754	41.989	25.454	1.00 22.91	C
ATOM	4136	C	MET	B	572	30.117	40.358	22.625	1.00 20.33	C
ATOM	4137	O	MET	B	572	30.204	39.235	22.101	1.00 20.73	O
ATOM	4138	N	SER	B	573	30.373	41.470	21.941	1.00 18.39	N
ATOM	4139	CA	SER	B	573	30.735	41.412	20.528	1.00 21.31	C
ATOM	4140	CB	SER	B	573	30.747	42.839	19.939	1.00 25.35	C
ATOM	4141	OG	SER	B	573	31.143	42.855	18.581	1.00 27.38	O
ATOM	4142	C	SER	B	573	32.073	40.693	20.296	1.00 23.59	C
ATOM	4143	O	SER	B	573	32.231	39.962	19.324	1.00 21.82	O
ATOM	4144	N	ASP	B	574	33.043	40.889	21.176	1.00 22.93	N
ATOM	4145	CA	ASP	B	574	34.322	40.196	21.019	1.00 21.19	C
ATOM	4146	CB	ASP	B	574	35.363	40.684	22.039	1.00 21.91	C
ATOM	4147	CG	ASP	B	574	35.914	42.071	21.707	1.00 25.96	C
ATOM	4148	OD1	ASP	B	574	35.752	42.553	20.567	1.00 23.74	O
ATOM	4149	OD2	ASP	B	574	36.547	42.657	22.604	1.00 26.12	O
ATOM	4150	C	ASP	B	574	34.156	38.667	21.166	1.00 22.88	C
ATOM	4151	O	ASP	B	574	34.942	37.915	20.585	1.00 23.63	O
ATOM	4152	N	CYS	B	575	33.161	38.218	21.938	1.00 19.59	N
ATOM	4153	CA	CYS	B	575	32.906	36.778	22.097	1.00 20.12	C
ATOM	4154	CB	CYS	B	575	31.822	36.522	23.163	1.00 22.35	C
ATOM	4155	SG	CYS	B	575	32.353	36.912	24.873	1.00 23.15	S
ATOM	4156	C	CYS	B	575	32.426	36.205	20.772	1.00 22.05	C
ATOM	4157	O	CYS	B	575	32.442	34.991	20.572	1.00 19.70	O
ATOM	4158	N	TRP	B	576	32.001	37.096	19.877	1.00 20.34	N
ATOM	4159	CA	TRP	B	576	31.514	36.699	18.556	1.00 19.05	C
ATOM	4160	CB	TRP	B	576	30.184	37.393	18.208	1.00 19.93	C
ATOM	4161	CG	TRP	B	576	29.089	37.172	19.205	1.00 22.10	C
ATOM	4162	CD2	TRP	B	576	28.077	38.106	19.558	1.00 17.49	C
ATOM	4163	CE2	TRP	B	576	27.263	37.485	20.547	1.00 18.66	C
ATOM	4164	CE3	TRP	B	576	27.763	39.414	19.127	1.00 16.82	C
ATOM	4165	CD1	TRP	B	576	28.868	36.045	19.956	1.00 20.31	C
ATOM	4166	NE1	TRP	B	576	27.764	36.225	20.770	1.00 19.04	N
ATOM	4167	CZ2	TRP	B	576	26.158	38.130	21.122	1.00 19.31	C
ATOM	4168	CZ3	TRP	B	576	26.653	40.059	19.692	1.00 19.50	C
ATOM	4169	CH2	TRP	B	576	25.861	39.418	20.684	1.00 19.35	C
ATOM	4170	C	TRP	B	576	32.493	36.958	17.405	1.00 22.30	C
ATOM	4171	O	TRP	B	576	32.062	37.191	16.262	1.00 20.73	O
ATOM	4172	N	ILE	B	577	33.792	36.942	17.714	1.00 19.99	N
ATOM	4173	CA	ILE	B	577	34.826	37.103	16.689	1.00 21.32	C
ATOM	4174	CB	ILE	B	577	36.215	37.309	17.338	1.00 20.92	C
ATOM	4175	CG2	ILE	B	577	37.351	36.977	16.323	1.00 19.24	C
ATOM	4176	CG1	ILE	B	577	36.318	38.764	17.847	1.00 26.98	N
ATOM	4177	CD1	ILE	B	577	37.577	39.046	18.674	1.00 31.70	C
ATOM	4178	C	ILE	B	577	34.774	35.798	15.891	1.00 22.46	C

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ATOM	4179	O	ILE	B	577	34.789	34.707	16.468	1.00	22.10	O
ATOM	4180	N	TYR	B	578	34.673	35.914	14.571	1.00	20.33	N
ATOM	4181	CA	TYR	B	578	34.532	34.751	13.715	1.00	24.28	C
ATOM	4182	CB	TYR	B	578	34.387	35.200	12.248	1.00	24.92	C
ATOM	4183	CG	TYR	B	578	33.925	34.103	11.307	1.00	25.66	C
ATOM	4184	CD1	TYR	B	578	32.574	33.963	10.977	1.00	29.87	C
ATOM	4185	CE1	TYR	B	578	32.139	32.918	10.134	1.00	32.04	C
ATOM	4186	CD2	TYR	B	578	34.831	33.173	10.770	1.00	31.85	C
ATOM	4187	CE2	TYR	B	578	34.397	32.126	9.938	1.00	29.55	C
ATOM	4188	CZ	TYR	B	578	33.047	32.009	9.628	1.00	31.34	C
ATOM	4189	OH	TYR	B	578	32.596	30.972	8.824	1.00	31.73	O
ATOM	4190	C	TYR	B	578	35.648	33.715	13.814	1.00	29.60	C
ATOM	4191	O	TYR	B	578	35.377	32.529	14.014	1.00	21.86	O
ATOM	4192	N	LYS	B	579	36.887	34.175	13.614	1.00	24.49	N
ATOM	4193	CA	LYS	B	579	38.069	33.335	13.631	1.00	27.75	C
ATOM	4194	CB	LYS	B	579	39.301	34.121	13.145	1.00	30.85	C
ATOM	4195	CG	LYS	B	579	39.212	34.623	11.695	1.00	39.76	C
ATOM	4196	CD	LYS	B	579	40.550	35.234	11.213	1.00	43.80	C
ATOM	4197	CE	LYS	B	579	40.481	35.643	9.735	1.00	52.66	C
ATOM	4198	NZ	LYS	B	579	41.684	36.457	9.328	1.00	53.08	N
ATOM	4199	C	LYS	B	579	38.346	32.811	15.021	1.00	28.50	C
ATOM	4200	O	LYS	B	579	38.585	33.568	15.942	1.00	27.27	O
ATOM	4201	N	TRP	B	580	38.335	31.495	15.128	1.00	27.56	N
ATOM	4202	CA	TRP	B	580	38.574	30.806	16.385	1.00	33.99	C
ATOM	4203	CB	TRP	B	580	38.649	29.310	16.079	1.00	33.38	C
ATOM	4204	CG	TRP	B	580	38.850	28.472	17.259	1.00	38.62	C
ATOM	4205	CD2	TRP	B	580	40.063	27.818	17.639	1.00	38.34	C
ATOM	4206	CE2	TRP	B	580	39.793	27.097	18.830	1.00	42.10	C
ATOM	4207	CE3	TRP	B	580	41.354	27.768	17.091	1.00	43.21	C
ATOM	4208	CD1	TRP	B	580	37.920	28.145	18.199	1.00	40.63	C
ATOM	4209	NE1	TRP	B	580	38.479	27.312	19.150	1.00	37.48	N
ATOM	4210	CZ2	TRP	B	580	40.767	26.333	19.484	1.00	42.20	C
ATOM	4211	CZ3	TRP	B	580	42.328	27.004	17.742	1.00	44.42	C
ATOM	4212	CH2	TRP	B	580	42.025	26.297	18.927	1.00	49.85	C
ATOM	4213	C	TRP	B	580	39.862	31.267	17.077	1.00	29.68	C
ATOM	4214	O	TRP	B	580	39.862	31.591	18.262	1.00	30.01	O
ATOM	4215	N	GLU	B	581	40.962	31.306	16.336	1.00	27.48	N
ATOM	4216	CA	GLU	B	581	42.236	31.710	16.917	1.00	27.95	C
ATOM	4217	CB	GLU	B	581	43.349	31.535	15.875	1.00	41.30	C
ATOM	4218	CG	GLU	B	581	43.080	30.409	14.878	1.00	45.98	C
ATOM	4219	CD	GLU	B	581	42.292	30.894	13.672	1.00	53.35	C
ATOM	4220	OE1	GLU	B	581	42.833	31.742	12.919	1.00	61.50	O
ATOM	4221	OE2	GLU	B	581	41.144	30.442	13.466	1.00	44.26	O
ATOM	4222	C	GLU	B	581	42.269	33.141	17.458	1.00	31.33	C
ATOM	4223	O	GLU	B	581	43.070	33.449	18.327	1.00	33.50	O
ATOM	4224	N	ASP	B	582	41.386	34.006	16.961	1.00	28.16	N
ATOM	4225	CA	ASP	B	582	41.341	35.407	17.389	1.00	24.75	C
ATOM	4226	CB	ASP	B	582	41.073	36.298	16.169	1.00	29.45	C
ATOM	4227	CG	ASP	B	582	42.179	36.201	15.131	1.00	39.01	C
ATOM	4228	OD1	ASP	B	582	43.301	35.821	15.524	1.00	35.67	O
ATOM	4229	OD2	ASP	B	582	41.937	36.495	13.937	1.00	38.00	O
ATOM	4230	C	ASP	B	582	40.307	35.726	18.478	1.00	26.77	C
ATOM	4231	O	ASP	B	582	40.250	36.848	18.993	1.00	25.92	O
ATOM	4232	N	ARG	B	583	39.487	34.744	18.816	1.00	27.16	N
ATOM	4233	CA	ARG	B	583	38.448	34.959	19.818	1.00	29.93	C
ATOM	4234	CB	ARG	B	583	37.324	33.921	19.611	1.00	23.20	C
ATOM	4235	CG	ARG	B	583	35.974	34.196	20.334	1.00	20.53	C
ATOM	4236	CD	ARG	B	583	34.993	33.051	20.050	1.00	17.55	C
ATOM	4237	NE	ARG	B	583	34.872	32.798	18.608	1.00	17.49	N
ATOM	4238	CZ	ARG	B	583	34.658	31.610	18.055	1.00	22.33	C
ATOM	4239	NH1	ARG	B	583	34.528	30.522	18.811	1.00	20.02	N
ATOM	4240	NH2	ARG	B	583	34.618	31.501	16.721	1.00	21.31	N
ATOM	4241	C	ARG	B	583	39.101	34.827	21.203	1.00	26.43	C
ATOM	4242	O	ARG	B	583	39.964	33.975	21.417	1.00	24.85	O
ATOM	4243	N	PRO	B	584	38.694	35.679	22.159	1.00	23.83	N
ATOM	4244	CD	PRO	B	584	37.731	36.791	22.028	1.00	23.73	C
ATOM	4245	CA	PRO	B	584	39.252	35.638	23.516	1.00	25.03	C
ATOM	4246	CB	PRO	B	584	38.660	36.877	24.178	1.00	25.59	C

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ATOM   4247  CG   PRO B 584      37.346  37.053  23.469  1.00 24.23           C
ATOM   4248  C    PRO B 584      38.890  34.383  24.302  1.00 25.66           C
ATOM   4249  O    PRO B 584      37.896  33.722  23.987  1.00 22.86           O
ATOM   4250  N    ASP B 585      39.714  34.082  25.314  1.00 20.92           N
ATOM   4251  CA   ASP B 585      39.492  32.946  26.205  1.00 23.08           C
ATOM   4252  CB   ASP B 585      40.833  32.346  26.685  1.00 32.60           C
ATOM   4253  CG   ASP B 585      41.670  31.806  25.541  1.00 38.55           C
ATOM   4254  OD1  ASP B 585      41.153  31.012  24.727  1.00 48.57           O
ATOM   4255  OD2  ASP B 585      42.865  32.180  25.469  1.00 55.39           O
ATOM   4256  C    ASP B 585      38.763  33.456  27.448  1.00 20.51           C
ATOM   4257  O    ASP B 585      38.686  34.667  27.668  1.00 23.27           O
ATOM   4258  N    PHE B 586      38.260  32.542  28.286  1.00 21.45           N
ATOM   4259  CA   PHE B 586      37.538  32.967  29.485  1.00 26.29           C
ATOM   4260  CB   PHE B 586      36.795  31.794  30.151  1.00 22.81           C
ATOM   4261  CG   PHE B 586      35.482  31.470  29.484  1.00 22.63           C
ATOM   4262  CD1  PHE B 586      34.406  32.367  29.542  1.00 24.53           C
ATOM   4263  CD2  PHE B 586      35.323  30.268  28.785  1.00 26.40           C
ATOM   4264  CE1  PHE B 586      33.179  32.049  28.910  1.00 18.28           C
ATOM   4265  CE2  PHE B 586      34.112  29.961  28.161  1.00 24.68           C
ATOM   4266  CZ   PHE B 586      33.048  30.847  28.231  1.00 19.51           C
ATOM   4267  C    PHE B 586      38.440  33.673  30.486  1.00 24.38           C
ATOM   4268  O    PHE B 586      37.983  34.473  31.267  1.00 23.72           O
ATOM   4269  N    LEU B 587      39.741  33.395  30.440  1.00 27.00           N
ATOM   4270  CA   LEU B 587      40.650  34.114  31.337  1.00 24.91           C
ATOM   4271  CB   LEU B 587      42.093  33.688  31.039  1.00 32.67           C
ATOM   4272  CG   LEU B 587      43.216  34.188  31.943  1.00 40.26           C
ATOM   4273  CD1  LEU B 587      43.348  35.672  31.784  1.00 43.71           C
ATOM   4274  CD2  LEU B 587      42.926  33.834  33.380  1.00 40.03           C
ATOM   4275  C    LEU B 587      40.455  35.627  31.106  1.00 23.16           C
ATOM   4276  O    LEU B 587      40.225  36.374  32.063  1.00 26.74           O
ATOM   4277  N    THR B 588      40.494  36.088  29.852  1.00 23.64           N
ATOM   4278  CA   THR B 588      40.294  37.516  29.607  1.00 22.82           C
ATOM   4279  CB   THR B 588      40.852  37.982  28.229  1.00 33.41           C
ATOM   4280  OG1  THR B 588      40.043  37.479  27.172  1.00 46.39           O
ATOM   4281  CG2  THR B 588      42.266  37.477  28.056  1.00 31.62           C
ATOM   4282  C    THR B 588      38.832  37.929  29.711  1.00 22.83           C
ATOM   4283  O    THR B 588      38.539  39.006  30.205  1.00 27.35           O
ATOM   4284  N    VAL B 589      37.915  37.069  29.258  1.00 23.23           N
ATOM   4285  CA   VAL B 589      36.502  37.418  29.370  1.00 23.31           C
ATOM   4286  CB   VAL B 589      35.601  36.298  28.759  1.00 25.23           C
ATOM   4287  CG1  VAL B 589      34.128  36.521  29.142  1.00 24.91           C
ATOM   4288  CG2  VAL B 589      35.751  36.315  27.238  1.00 24.02           C
ATOM   4289  C    VAL B 589      36.082  37.688  30.816  1.00 21.77           C
ATOM   4290  O    VAL B 589      35.384  38.666  31.097  1.00 21.67           O
ATOM   4291  N    GLU B 590      36.503  36.817  31.736  1.00 24.09           N
ATOM   4292  CA   GLU B 590      36.158  36.986  33.149  1.00 23.44           C
ATOM   4293  CB   GLU B 590      36.700  35.792  33.980  1.00 23.66           C
ATOM   4294  CG   GLU B 590      36.346  35.806  35.489  1.00 28.31           C
ATOM   4295  CD   GLU B 590      37.173  36.793  36.342  1.00 30.31           C
ATOM   4296  OE1  GLU B 590      38.375  36.990  36.060  1.00 30.33           O
ATOM   4297  OE2  GLU B 590      36.623  37.345  37.325  1.00 30.51           O
ATOM   4298  C    GLU B 590      36.722  38.300  33.698  1.00 24.63           C
ATOM   4299  O    GLU B 590      36.060  38.995  34.469  1.00 21.17           O
ATOM   4300  N    GLN B 591      37.948  38.645  33.304  1.00 23.83           N
ATOM   4301  CA   GLN B 591      38.550  39.896  33.775  1.00 25.38           C
ATOM   4302  CB   GLN B 591      40.005  39.980  33.324  1.00 27.76           C
ATOM   4303  CG   GLN B 591      40.877  38.896  33.902  1.00 36.74           C
ATOM   4304  CD   GLN B 591      42.333  39.101  33.554  1.00 43.26           C
ATOM   4305  OE1  GLN B 591      42.669  39.908  32.677  1.00 44.86           O
ATOM   4306  NE2  GLN B 591      43.206  38.370  34.230  1.00 44.68           N
ATOM   4307  C    GLN B 591      37.818  41.132  33.279  1.00 25.08           C
ATOM   4308  O    GLN B 591      37.616  42.102  34.019  1.00 26.57           O
ATOM   4309  N    ARG B 592      37.423  41.110  32.012  1.00 23.67           N
ATOM   4310  CA   ARG B 592      36.712  42.239  31.437  1.00 25.80           C
ATOM   4311  CB   ARG B 592      36.631  42.087  29.917  1.00 23.30           C
ATOM   4312  CG   ARG B 592      38.018  42.247  29.276  1.00 31.02           C
ATOM   4313  CD   ARG B 592      38.006  41.980  27.792  1.00 31.50           C
ATOM   4314  NE   ARG B 592      37.163  42.935  27.079  1.00 25.46           N
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ATOM	4315	CZ	ARG	B	592	36.913	42.861	25.781	1.00	24.58	C
ATOM	4316	NH1	ARG	B	592	37.446	41.880	25.069	1.00	25.78	N
ATOM	4317	NH2	ARG	B	592	36.127	43.760	25.206	1.00	26.82	N
ATOM	4318	C	ARG	B	592	35.326	42.323	32.039	1.00	25.35	C
ATOM	4319	O	ARG	B	592	34.803	43.415	32.284	1.00	25.98	O
ATOM	4320	N	MET	B	593	34.722	41.165	32.293	1.00	23.15	N
ATOM	4321	CA	MET	B	593	33.380	41.176	32.867	1.00	24.63	C
ATOM	4322	CB	MET	B	593	32.774	39.764	32.822	1.00	22.51	C
ATOM	4323	CG	MET	B	593	31.324	39.697	33.218	1.00	22.94	C
ATOM	4324	SD	MET	B	593	30.230	40.679	32.086	1.00	29.24	S
ATOM	4325	CE	MET	B	593	29.463	41.710	33.269	1.00	27.63	C
ATOM	4326	C	MET	B	593	33.442	41.705	34.297	1.00	25.96	C
ATOM	4327	O	MET	B	593	32.582	42.480	34.719	1.00	28.48	O
ATOM	4328	N	ARG	B	594	34.459	41.296	35.044	1.00	23.96	N
ATOM	4329	CA	ARG	B	594	34.605	41.743	36.417	1.00	24.96	C
ATOM	4330	CB	ARG	B	594	35.849	41.106	37.042	1.00	23.17	C
ATOM	4331	CG	ARG	B	594	36.061	41.480	38.522	1.00	25.85	C
ATOM	4332	CD	ARG	B	594	37.401	40.946	39.044	1.00	37.38	C
ATOM	4333	NE	ARG	B	594	37.415	39.490	39.157	1.00	42.96	N
ATOM	4334	CZ	ARG	B	594	36.932	38.814	40.201	1.00	43.14	C
ATOM	4335	NH1	ARG	B	594	36.400	39.464	41.232	1.00	47.77	N
ATOM	4336	NH2	ARG	B	594	36.966	37.488	40.206	1.00	41.23	N
ATOM	4337	C	ARG	B	594	34.707	43.271	36.461	1.00	27.20	C
ATOM	4338	O	ARG	B	594	34.071	43.930	37.291	1.00	29.00	O
ATOM	4339	N	ALA	B	595	35.499	43.827	35.548	1.00	29.98	N
ATOM	4340	CA	ALA	B	595	35.709	45.271	35.455	1.00	32.90	C
ATOM	4341	CB	ALA	B	595	36.814	45.570	34.424	1.00	33.21	C
ATOM	4342	C	ALA	B	595	34.423	46.010	35.087	1.00	33.52	C
ATOM	4343	O	ALA	B	595	34.139	47.075	35.627	1.00	31.72	O
ATOM	4344	N	CYS	B	596	33.646	45.439	34.166	1.00	31.09	N
ATOM	4345	CA	CYS	B	596	32.389	46.044	33.750	1.00	32.73	C
ATOM	4346	CB	CYS	B	596	31.768	45.264	32.585	1.00	31.31	C
ATOM	4347	SG	CYS	B	596	32.614	45.490	30.999	1.00	41.27	S
ATOM	4348	C	CYS	B	596	31.412	46.053	34.907	1.00	33.26	C
ATOM	4349	O	CYS	B	596	30.741	47.055	35.158	1.00	31.15	O
ATOM	4350	N	TYR	B	597	31.326	44.925	35.604	1.00	28.78	N
ATOM	4351	CA	TYR	B	597	30.415	44.811	36.736	1.00	29.03	C
ATOM	4352	CB	TYR	B	597	30.465	43.384	37.311	1.00	30.58	C
ATOM	4353	CG	TYR	B	597	29.811	43.233	38.665	1.00	31.39	C
ATOM	4354	CD1	TYR	B	597	28.548	43.773	38.917	1.00	33.23	C
ATOM	4355	CE1	TYR	B	597	27.957	43.673	40.186	1.00	36.25	C
ATOM	4356	CD2	TYR	B	597	30.465	42.579	39.702	1.00	36.29	C
ATOM	4357	CE2	TYR	B	597	29.884	42.466	40.977	1.00	42.36	C
ATOM	4358	CZ	TYR	B	597	28.634	43.021	41.210	1.00	40.23	C
ATOM	4359	OH	TYR	B	597	28.091	42.957	42.474	1.00	40.28	O
ATOM	4360	C	TYR	B	597	30.758	45.825	37.827	1.00	32.53	C
ATOM	4361	O	TYR	B	597	29.871	46.537	38.335	1.00	33.59	O
ATOM	4362	N	TYR	B	598	32.036	45.883	38.179	1.00	30.77	N
ATOM	4363	CA	TYR	B	598	32.508	46.793	39.218	1.00	38.97	C
ATOM	4364	CB	TYR	B	598	34.012	46.604	39.460	1.00	39.06	C
ATOM	4365	CG	TYR	B	598	34.385	45.365	40.244	1.00	40.81	C
ATOM	4366	CD1	TYR	B	598	35.714	45.111	40.590	1.00	48.71	C
ATOM	4367	CE1	TYR	B	598	36.075	43.943	41.281	1.00	48.51	C
ATOM	4368	CD2	TYR	B	598	33.424	44.423	40.612	1.00	47.38	C
ATOM	4369	CE2	TYR	B	598	33.771	43.259	41.298	1.00	46.97	C
ATOM	4370	CZ	TYR	B	598	35.098	43.024	41.626	1.00	49.34	C
ATOM	4371	OH	TYR	B	598	35.445	41.854	42.264	1.00	48.67	O
ATOM	4372	C	TYR	B	598	32.227	48.230	38.823	1.00	43.37	C
ATOM	4373	O	TYR	B	598	31.873	49.057	39.667	1.00	48.95	O
ATOM	4374	N	SER	B	599	32.379	48.535	37.541	1.00	37.43	N
ATOM	4375	CA	SER	B	599	32.122	49.872	37.055	1.00	43.16	C
ATOM	4376	CB	SER	B	599	32.529	49.961	35.590	1.00	43.45	C
ATOM	4377	OG	SER	B	599	32.332	51.262	35.090	1.00	53.97	O
ATOM	4378	C	SER	B	599	30.636	50.205	37.223	1.00	45.93	C
ATOM	4379	O	SER	B	599	30.271	51.316	37.617	1.00	40.00	O
ATOM	4380	N	LEU	B	600	29.773	49.240	36.935	1.00	39.11	N
ATOM	4381	CA	LEU	B	600	28.337	49.462	37.065	1.00	44.57	C
ATOM	4382	CB	LEU	B	600	27.552	48.395	36.295	1.00	38.25	C

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ATOM   4383  CG  LEU B 600      27.711  48.441  34.770  1.00 42.03           C
ATOM   4384  CD1 LEU B 600      27.111  47.196  34.147  1.00 37.50           C
ATOM   4385  CD2 LEU B 600      27.039  49.683  34.214  1.00 45.85           C
ATOM   4386  C   LEU B 600      27.897  49.456  38.516  1.00 43.73           C
ATOM   4387  O   LEU B 600      26.980  50.191  38.892  1.00 46.87           O
ATOM   4388  N   ALA B 601      28.556  48.628  39.323  1.00 40.69           N
ATOM   4389  CA  ALA B 601      28.242  48.478  40.741  1.00 47.37           C
ATOM   4390  CB  ALA B 601      29.065  47.346  41.335  1.00 46.75           C
ATOM   4391  C   ALA B 601      28.506  49.775  41.498  1.00 52.65           C
ATOM   4392  O   ALA B 601      27.834  50.082  42.483  1.00 53.31           O
ATOM   4393  N   SER B 602      29.492  50.527  41.021  1.00 52.09           N
ATOM   4394  CA  SER B 602      29.860  51.804  41.617  1.00 57.33           C
ATOM   4395  CB  SER B 602      31.346  52.069  41.381  1.00 58.94           C
ATOM   4396  OG  SER B 602      32.141  51.082  42.020  1.00 59.82           O
ATOM   4397  C   SER B 602      29.024  52.912  40.981  1.00 59.94           C
ATOM   4398  O   SER B 602      29.388  54.086  41.029  1.00 64.66           O
ATOM   4399  N   LYS B 603      27.900  52.515  40.389  1.00 62.33           N
ATOM   4400  CA  LYS B 603      26.974  53.425  39.720  1.00 64.02           C
ATOM   4401  CB  LYS B 603      26.569  54.555  40.673  1.00 64.16           C
ATOM   4402  CG  LYS B 603      25.091  54.908  40.626  1.00 65.22           C
ATOM   4403  CD  LYS B 603      24.767  55.995  41.635  1.00 64.28           C
ATOM   4404  CE  LYS B 603      23.270  56.270  41.693  1.00 67.89           C
ATOM   4405  NZ  LYS B 603      22.949  57.422  42.589  1.00 67.06           N
ATOM   4406  C   LYS B 603      27.609  53.996  38.446  1.00 65.47           C
ATOM   4407  O   LYS B 603      27.032  53.798  37.352  1.00 66.51           O
ATOM   4408  OXT LYS B 603      28.685  54.625  38.551  1.00 68.34           O
TER       1      LYS B 603
ATOM   4409  O4  STU C 995      10.701  -7.072  -3.088  1.00 26.93           O
ATOM   4410  C25 STU C 995      11.180  -5.863  -3.690  1.00 23.34           C
ATOM   4411  C24 STU C 995      10.859  -4.664  -2.680  1.00 29.45           C
ATOM   4412  C23 STU C 995      10.138  -5.127  -1.364  1.00 22.89           C
ATOM   4413  C22 STU C 995       8.878  -5.986  -1.697  1.00 25.16           C
ATOM   4414  C21 STU C 995       9.461  -7.275  -2.433  1.00 26.44           C
ATOM   4415  C26 STU C 995       9.777  -8.334  -1.360  1.00 25.18           C
ATOM   4416  N2  STU C 995       8.422  -7.719  -3.422  1.00 23.09           N
ATOM   4417  C18 STU C 995       8.412  -7.138  -4.747  1.00 21.71           C
ATOM   4418  C19 STU C 995       9.290  -6.274  -5.405  1.00 24.08           C
ATOM   4419  C6  STU C 995       9.064  -5.832  -6.736  1.00 22.57           C
ATOM   4420  C7  STU C 995       7.866  -6.422  -7.405  1.00 25.97           C
ATOM   4421  C10 STU C 995       7.050  -7.293  -6.788  1.00 23.03           C
ATOM   4422  C11 STU C 995       7.275  -7.726  -5.438  1.00 20.70           C
ATOM   4423  C12 STU C 995       6.603  -8.591  -4.523  1.00 24.72           C
ATOM   4424  C17 STU C 995       7.298  -8.588  -3.264  1.00 25.22           C
ATOM   4425  C16 STU C 995       6.820  -9.373  -2.193  1.00 26.63           C
ATOM   4426  C15 STU C 995       5.671 -10.131  -2.339  1.00 28.90           C
ATOM   4427  C14 STU C 995       4.957 -10.136  -3.585  1.00 27.59           C
ATOM   4428  C13 STU C 995       5.443  -9.364  -4.643  1.00 24.26           C
ATOM   4429  C9  STU C 995       5.906  -7.701  -7.728  1.00 24.86           C
ATOM   4430  N1  STU C 995       6.283  -6.914  -8.894  1.00 26.80           N
ATOM   4431  C8  STU C 995       7.390  -6.161  -8.794  1.00 24.42           C
ATOM   4432  O5  STU C 995       7.870  -5.431  -9.638  1.00 25.22           O
ATOM   4433  C5  STU C 995      10.084  -4.899  -7.090  1.00 21.94           C
ATOM   4434  C20 STU C 995      10.927  -4.761  -5.943  1.00 28.12           C
ATOM   4435  C1  STU C 995      12.071  -3.894  -5.922  1.00 27.73           C
ATOM   4436  C2  STU C 995      12.350  -3.175  -7.097  1.00 30.27           C
ATOM   4437  C3  STU C 995      11.500  -3.313  -8.263  1.00 28.96           C
ATOM   4438  C4  STU C 995      10.403  -4.161  -8.243  1.00 26.89           C
ATOM   4439  N3  STU C 995      10.433  -5.565  -4.940  1.00 23.33           N
ATOM   4440  O6  STU C 995       8.116  -5.181  -2.652  1.00 24.62           O
ATOM   4441  C27 STU C 995       6.704  -5.144  -2.385  1.00 24.32           C
ATOM   4442  N4  STU C 995       9.777  -3.833  -0.560  1.00 24.88           N
ATOM   4443  C28 STU C 995       9.296  -4.199   0.820  1.00 26.60           C
TER       1      STU C 995
ATOM   4444  O4  STU D 996      14.841  21.718  34.032  1.00 26.13           O
ATOM   4445  C25 STU D 996      14.373  22.920  34.632  1.00 22.93           C
ATOM   4446  C24 STU D 996      14.706  24.128  33.610  1.00 28.10           C
ATOM   4447  C23 STU D 996      15.417  23.644  32.288  1.00 24.94           C
ATOM   4448  C22 STU D 996      16.665  22.776  32.631  1.00 23.21           C
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ATOM   4449   C21  STU D 996      16.072   21.495   33.377   1.00  27.43        C
ATOM   4450   C26  STU D 996      15.756   20.434   32.323   1.00  26.04        C
ATOM   4451   N2   STU D 996      17.133   21.077   34.359   1.00  21.43        N
ATOM   4452   C18  STU D 996      17.120   21.637   35.688   1.00  20.69        C
ATOM   4453   C19  STU D 996      16.275   22.524   36.330   1.00  23.53        C
ATOM   4454   C6   STU D 996      16.487   22.957   37.663   1.00  22.38        C
ATOM   4455   C7   STU D 996      17.682   22.366   38.337   1.00  26.78        C
ATOM   4456   C10  STU D 996      18.504   21.518   37.720   1.00  22.89        C
ATOM   4457   C11  STU D 996      18.270   21.070   36.370   1.00  19.86        C
ATOM   4458   C12  STU D 996      18.952   20.227   35.457   1.00  22.51        C
ATOM   4459   C17  STU D 996      18.237   20.202   34.206   1.00  25.41        C
ATOM   4460   C16  STU D 996      18.719   19.424   33.133   1.00  26.19        C
ATOM   4461   C15  STU D 996      19.869   18.670   33.275   1.00  28.16        C
ATOM   4462   C14  STU D 996      20.600   18.678   34.521   1.00  25.48        C
ATOM   4463   C13  STU D 996      20.112   19.449   35.580   1.00  23.07        C
ATOM   4464   C9   STU D 996      19.647   21.104   38.659   1.00  23.46        C
ATOM   4465   N1   STU D 996      19.276   21.887   39.826   1.00  25.16        N
ATOM   4466   C8   STU D 996      18.166   22.640   39.728   1.00  22.97        C
ATOM   4467   O5   STU D 996      17.688   23.365   40.576   1.00  23.93        O
ATOM   4468   C5   STU D 996      15.472   23.870   38.015   1.00  23.02        C
ATOM   4469   C20  STU D 996      14.631   24.010   36.865   1.00  26.41        C
ATOM   4470   C1   STU D 996      13.476   24.883   36.850   1.00  25.65        C
ATOM   4471   C2   STU D 996      13.208   25.595   38.019   1.00  30.69        C
ATOM   4472   C3   STU D 996      14.057   25.459   39.181   1.00  27.27        C
ATOM   4473   C4   STU D 996      15.157   24.612   39.158   1.00  26.75        C
ATOM   4474   N3   STU D 996      15.112   23.212   35.878   1.00  22.92        N
ATOM   4475   O6   STU D 996      17.429   23.573   33.576   1.00  23.16        O
ATOM   4476   C27  STU D 996      18.832   23.642   33.286   1.00  24.37        C
ATOM   4477   N4   STU D 996      15.802   24.935   31.463   1.00  23.94        N
ATOM   4478   C28  STU D 996      16.275   24.547   30.090   1.00  24.01        C
TER    1          STU D 996
ATOM   4479   OH2  TIP S   1       0.421    4.204   13.673   1.00  22.10        O
ATOM   4480   OH2  TIP S   2       0.033    9.184   13.707   1.00  21.18        O
ATOM   4481   OH2  TIP S   3      11.945   -2.213    0.210   1.00  22.87        O
ATOM   4482   OH2  TIP S   4      25.132   33.017   17.239   1.00  22.45        O
ATOM   4483   OH2  TIP S   5      25.496   37.992   17.154   1.00  20.79        O
ATOM   4484   OH2  TIP S   6     -12.049  -13.944   12.451   1.00  22.33        O
ATOM   4485   OH2  TIP S   7      14.395    8.858   57.889   1.00  29.61        O
ATOM   4486   OH2  TIP S   8      13.627   26.578   30.735   1.00  22.89        O
ATOM   4487   OH2  TIP S   9      11.059  -19.955  -26.913   1.00  28.80        O
ATOM   4488   OH2  TIP S  10      29.070   27.910   20.630   1.00  25.77        O
ATOM   4489   OH2  TIP S  11      -3.520   -0.809   10.277   1.00  25.06        O
ATOM   4490   OH2  TIP S  12      18.345   30.239   26.486   1.00  23.39        O
ATOM   4491   OH2  TIP S  13       1.869   14.815   18.471   1.00  23.60        O
ATOM   4492   OH2  TIP S  14      35.075   25.727   28.589   1.00  28.87        O
ATOM   4493   OH2  TIP S  15       7.227    1.385    4.419   1.00  22.68        O
ATOM   4494   OH2  TIP S  16      -9.560   -3.026    2.397   1.00  27.48        O
ATOM   4495   OH2  TIP S  17      -5.464   -3.857    7.924   1.00  23.68        O
ATOM   4496   OH2  TIP S  18      -6.496    8.745   20.202   1.00  23.82        O
ATOM   4497   OH2  TIP S  19      -2.873   -2.292    5.603   1.00  23.16        O
ATOM   4498   OH2  TIP S  20     -11.803    8.285   18.254   1.00  24.29        O
ATOM   4499   OH2  TIP S  21      28.416   26.453   25.290   1.00  23.25        O
ATOM   4500   OH2  TIP S  22      37.391   37.035   12.669   1.00  26.06        O
ATOM   4501   OH2  TIP S  23     -17.573   -7.098    4.343   1.00  27.79        O
ATOM   4502   OH2  TIP S  24      32.073   37.514   10.731   1.00  24.94        O
ATOM   4503   OH2  TIP S  25      13.480   31.449   36.563   1.00  25.71        O
ATOM   4504   OH2  TIP S  26     -14.437    9.362   17.730   1.00  32.36        O
ATOM   4505   OH2  TIP S  27      35.416   25.457   18.662   1.00  25.28        O
ATOM   4506   OH2  TIP S  28      31.029   24.811   22.942   1.00  25.60        O
ATOM   4507   OH2  TIP S  29      -9.872   -3.294   12.263   1.00  25.74        O
ATOM   4508   OH2  TIP S  30      26.467    9.752   17.607   1.00  27.17        O
ATOM   4509   OH2  TIP S  31       6.790   -6.857    1.076   1.00  30.39        O
ATOM   4510   OH2  TIP S  32      40.010   38.095   13.209   1.00  33.16        O
ATOM   4511   OH2  TIP S  33      34.735   13.425   28.194   1.00  29.80        O
ATOM   4512   OH2  TIP S  34      -9.205  -15.364    2.764   1.00  26.99        O
ATOM   4513   OH2  TIP S  35      -0.980  -18.986   13.270   1.00  26.43        O
ATOM   4514   OH2  TIP S  36      24.213   18.114   34.694   1.00  29.43        O
ATOM   4515   OH2  TIP S  37       1.416  -10.764   -3.798   1.00  29.81        O
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ATOM    4516  OH2 TIP S  38      43.144   21.699   26.548  1.00 30.26         O
ATOM    4517  OH2 TIP S  39     -14.848    7.171   -3.854  1.00 30.65         O
ATOM    4518  OH2 TIP S  40      39.180   42.936   36.141  1.00 31.31         O
ATOM    4519  OH2 TIP S  41      40.406   35.919   34.784  1.00 30.00         O
ATOM    4520  OH2 TIP S  42       0.420    2.218   15.485  1.00 29.77         O
ATOM    4521  OH2 TIP S  43      35.271   29.926   13.265  1.00 31.24         O
ATOM    4522  OH2 TIP S  44      12.095    2.647   -5.592  1.00 26.76         O
ATOM    4523  OH2 TIP S  45      -9.718    1.172   17.653  1.00 30.07         O
ATOM    4524  OH2 TIP S  46      -3.404   14.594   13.732  1.00 30.39         O
ATOM    4525  OH2 TIP S  47      18.726   21.922   29.867  1.00 32.07         O
ATOM    4526  OH2 TIP S  48      13.555    7.866   51.920  1.00 39.23         O
ATOM    4527  OH2 TIP S  49      28.975   43.404   17.200  1.00 29.02         O
ATOM    4528  OH2 TIP S  50     -13.569   14.156   -5.246  1.00 33.70         O
ATOM    4529  OH2 TIP S  51      26.355   20.255   28.832  1.00 29.58         O
ATOM    4530  OH2 TIP S  52       9.161   10.323   16.585  1.00 35.40         O
ATOM    4531  OH2 TIP S  53      -0.757   -8.626    2.106  1.00 29.81         O
ATOM    4532  OH2 TIP S  54     -14.070   -4.107    6.620  1.00 27.24         O
ATOM    4533  OH2 TIP S  55      11.946  -20.893  -21.008  1.00 43.13         O
ATOM    4534  OH2 TIP S  56      25.189   30.969   15.454  1.00 29.79         O
ATOM    4535  OH2 TIP S  57      36.813   31.260   38.289  1.00 31.14         O
ATOM    4536  OH2 TIP S  58     -11.290    2.441   -7.391  1.00 30.15         O
ATOM    4537  OH2 TIP S  59       9.218   10.129   12.339  1.00 32.37         O
ATOM    4538  OH2 TIP S  60      16.469   39.110   14.335  1.00 36.98         O
ATOM    4539  OH2 TIP S  61      39.600   24.658   24.347  1.00 28.57         O
ATOM    4540  OH2 TIP S  62      40.886   19.814   39.523  1.00 31.30         O
ATOM    4541  OH2 TIP S  63      28.663   25.506   21.907  1.00 28.05         O
ATOM    4542  OH2 TIP S  64      16.334   39.034   18.587  1.00 30.97         O
ATOM    4543  OH2 TIP S  65      -4.453  -10.056  -10.600  1.00 35.01         O
ATOM    4544  OH2 TIP S  66      30.644   48.610   22.338  1.00 34.83         O
ATOM    4545  OH2 TIP S  67      29.080   17.008   23.184  1.00 42.53         O
ATOM    4546  OH2 TIP S  68      20.437   -8.985   -8.586  1.00 30.66         O
ATOM    4547  OH2 TIP S  69      -3.136   -3.317    8.937  1.00 26.92         O
ATOM    4548  OH2 TIP S  70      -3.528  -11.754    7.661  1.00 42.36         O
ATOM    4549  OH2 TIP S  71     -14.052    9.990   -6.784  1.00 36.91         O
ATOM    4550  OH2 TIP S  72      13.280   20.389   48.150  1.00 37.12         O
ATOM    4551  OH2 TIP S  73      39.598   27.291   23.321  1.00 29.86         O
ATOM    4552  OH2 TIP S  74     -14.000   -1.419    7.609  1.00 29.52         O
ATOM    4553  OH2 TIP S  75      12.287   -8.370  -17.212  1.00 38.16         O
ATOM    4554  OH2 TIP S  76       0.127   -2.062    7.336  1.00 31.92         O
ATOM    4555  OH2 TIP S  77      39.657   38.747   37.688  1.00 35.97         O
ATOM    4556  OH2 TIP S  78       6.921   10.871   13.240  1.00 39.95         O
ATOM    4557  OH2 TIP S  79       3.173   20.739   -5.925  1.00 36.12         O
ATOM    4558  OH2 TIP S  80       2.499   -2.849    7.192  1.00 37.12         O
ATOM    4559  OH2 TIP S  81      -5.087   20.010    8.545  1.00 36.89         O
ATOM    4560  OH2 TIP S  82      25.391   26.672   23.460  1.00 34.04         O
ATOM    4561  OH2 TIP S  83      23.029   25.932   23.668  1.00 37.18         O
ATOM    4562  OH2 TIP S  84      13.382   -6.941   -0.286  1.00 40.85         O
ATOM    4563  OH2 TIP S  85      27.715   12.569   29.074  1.00 44.29         O
ATOM    4564  OH2 TIP S  86      29.990   18.665   41.491  1.00 37.50         O
ATOM    4565  OH2 TIP S  87      22.380   49.448   36.934  1.00 39.98         O
ATOM    4566  OH2 TIP S  88      18.662   39.652   17.714  1.00 39.70         O
ATOM    4567  OH2 TIP S  89      40.100   17.469   30.708  1.00 36.01         O
ATOM    4568  OH2 TIP S  90     -14.239   11.528    5.631  1.00 40.89         O
ATOM    4569  OH2 TIP S  91      15.281   18.913   57.001  1.00 45.15         O
ATOM    4570  OH2 TIP S  92      15.691   -4.194   -6.244  1.00 46.89         O
ATOM    4571  OH2 TIP S  93      -5.712   -9.326    5.564  1.00 28.37         O
ATOM    4572  OH2 TIP S  94      12.167   21.855   31.241  1.00 41.68         O
ATOM    4573  OH2 TIP S  95      -3.343  -17.247   16.589  1.00 36.78         O
ATOM    4574  OH2 TIP S  96      11.156   23.711   33.209  1.00 35.57         O
ATOM    4575  OH2 TIP S  97      25.545   16.245   18.621  1.00 42.42         O
ATOM    4576  OH2 TIP S  98      40.918   18.920   34.722  1.00 45.15         O
ATOM    4577  OH2 TIP S  99      11.862   37.569   22.369  1.00 39.52         O
ATOM    4578  OH2 TIP S 100      15.658    8.162   -3.968  1.00 36.43         O
ATOM    4579  OH2 TIP S 101       9.902   24.553   37.142  1.00 45.39         O
ATOM    4580  OH2 TIP S 102       6.314   -5.317  -19.652  1.00 42.39         O
ATOM    4581  OH2 TIP S 103      41.337   39.304   18.249  1.00 43.68         O
ATOM    4582  OH2 TIP S 104       1.800   -8.520   -5.551  1.00 35.38         O
ATOM    4583  OH2 TIP S 105      -2.162  -16.185    1.874  1.00 43.33         O
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ATOM    4584   OH2 TIP S 106    39.849  40.296  25.274   1.00 39.96        O
ATOM    4585   OH2 TIP S 107    17.812  14.377  26.537   1.00 49.82        O
ATOM    4586   OH2 TIP S 108    20.087  16.149  58.833   1.00 41.90        O
ATOM    4587   OH2 TIP S 109    23.681  20.283  36.450   1.00 34.15        O
ATOM    4588   OH2 TIP S 110    31.232  19.396  25.383   1.00 31.15        O
ATOM    4589   OH2 TIP S 111     9.926  36.917  34.935   1.00 39.68        O
ATOM    4590   OH2 TIP S 112    13.742   8.657   8.468   1.00 37.13        O
ATOM    4591   OH2 TIP S 113    14.444  -5.155  -2.332   1.00 34.36        O
ATOM    4592   OH2 TIP S 114   -14.505 -11.350   0.205   1.00 38.40        O
ATOM    4593   OH2 TIP S 115   -14.458   0.142   5.499   1.00 35.12        O
ATOM    4594   OH2 TIP S 116    -0.021 -12.439  12.153   1.00 43.53        O
ATOM    4595   OH2 TIP S 117    28.916  11.485  14.387   1.00 40.27        O
ATOM    4596   OH2 TIP S 118    -4.527  10.289  -9.542   1.00 45.18        O
ATOM    4597   OH2 TIP S 119     1.974  14.755 -11.306   1.00 47.77        O
ATOM    4598   OH2 TIP S 120   -15.749  10.668  12.672   1.00 45.53        O
ATOM    4599   OH2 TIP S 121   -11.214  -2.226 -11.345   1.00 46.10        O
ATOM    4600   OH2 TIP S 122    36.682  45.523  28.569   1.00 37.78        O
ATOM    4601   OH2 TIP S 123    19.320  23.480  50.684   1.00 40.47        O
ATOM    4602   OH2 TIP S 124   -15.435  -9.919  -3.811   1.00 41.21        O
ATOM    4603   OH2 TIP S 125    38.588  26.717  13.793   1.00 44.52        O
ATOM    4604   OH2 TIP S 126     7.685 -14.424   4.306   1.00 51.58        O
ATOM    4605   OH2 TIP S 127    36.734  26.561  42.263   1.00 44.35        O
ATOM    4606   OH2 TIP S 128    23.012  18.699  64.427   1.00 55.43        O
ATOM    4607   OH2 TIP S 129   -11.079  16.753   2.337   1.00 36.15        O
ATOM    4608   OH2 TIP S 130    32.804  36.247   8.025   1.00 46.53        O
ATOM    4609   OH2 TIP S 131     5.452 -12.666 -27.857   1.00 46.24        O
ATOM    4610   OH2 TIP S 132     5.777  -5.213   4.878   1.00 52.94        O
ATOM    4611   OH2 TIP S 133    17.902  43.584  22.888   1.00 38.79        O
ATOM    4612   OH2 TIP S 134    41.529  41.359  30.489   1.00 45.08        O
ATOM    4613   OH2 TIP S 135    19.433  49.428  35.071   1.00 36.73        O
ATOM    4614   OH2 TIP S 136    40.681  17.939  17.861   1.00 52.60        O
ATOM    4615   OH2 TIP S 137     7.694  14.779   8.016   1.00 38.37        O
ATOM    4616   OH2 TIP S 138    43.631  21.569  35.087   1.00 42.92        O
ATOM    4617   OH2 TIP S 139   -14.096  -4.522   2.725   1.00 38.87        O
ATOM    4618   OH2 TIP S 140    39.647  24.357  28.138   1.00 37.44        O
ATOM    4619   OH2 TIP S 141    34.792  45.810  26.786   1.00 33.97        O
ATOM    4620   OH2 TIP S 142    35.678  30.939  40.741   1.00 50.18        O
ATOM    4621   OH2 TIP S 143     1.690  -5.943   7.932   1.00 46.04        O
ATOM    4622   OH2 TIP S 144    16.446   8.323  29.203   1.00 43.29        O
ATOM    4623   OH2 TIP S 145     4.806  -6.139 -16.268   1.00 46.89        O
ATOM    4624   OH2 TIP S 146     9.706   7.514 -13.847   1.00 40.39        O
ATOM    4625   OH2 TIP S 147    -2.757  -8.476  20.990   1.00 44.56        O
ATOM    4626   OH2 TIP S 148    19.924  51.030  32.912   1.00 56.09        O
ATOM    4627   OH2 TIP S 149    -9.256  17.012   4.187   1.00 37.40        O
ATOM    4628   OH2 TIP S 150    13.798  12.721   1.801   1.00 41.15        O
ATOM    4629   OH2 TIP S 151   -16.062  12.522   0.503   1.00 45.91        O
ATOM    4630   OH2 TIP S 152    43.042  24.814  30.118   1.00 45.63        O
ATOM    4631   OH2 TIP S 153    32.777  49.012  32.108   1.00 49.84        O
ATOM    4632   OH2 TIP S 154    35.924  45.614  31.001   1.00 42.83        O
ATOM    4633   OH2 TIP S 155    -4.339 -23.117  -0.551   1.00 49.33        O
ATOM    4634   OH2 TIP S 156    19.827  23.697  25.905   1.00 53.14        O
ATOM    4635   OH2 TIP S 157    37.820  44.919  22.145   1.00 44.38        O
ATOM    4636   OH2 TIP S 158    40.593  29.995  32.300   1.00 31.52        O
ATOM    4637   OH2 TIP S 159   -15.055   1.168  -1.359   1.00 30.62        O
ATOM    4638   OH2 TIP S 160   -16.412   7.003   5.433   1.00 32.94        O
ATOM    4639   OH2 TIP S 161    15.985  29.616  25.353   1.00 32.77        O
ATOM    4640   OH2 TIP S 162    42.076  35.832  25.453   1.00 35.51        O
ATOM    4641   OH2 TIP S 163    10.339  -9.751 -25.987   1.00 46.65        O
ATOM    4642   OH2 TIP S 164    34.356  38.780  10.727   1.00 36.90        O
ATOM    4643   OH2 TIP S 165     9.618   0.824   5.500   1.00 35.38        O
ATOM    4644   OH2 TIP S 166    26.940   9.884  20.217   1.00 38.88        O
ATOM    4645   OH2 TIP S 167    -7.023   7.631  22.982   1.00 45.13        O
ATOM    4646   OH2 TIP S 168   -17.523  -3.768   0.764   1.00 47.38        O
ATOM    4647   OH2 TIP S 169    34.610  28.019  11.023   1.00 41.98        O
ATOM    4648   OH2 TIP S 170    38.500  22.241  10.888   1.00 49.86        O
ATOM    4649   OH2 TIP S 171    39.773  16.186  22.302   1.00 42.81        O
ATOM    4650   OH2 TIP S 172    39.007  29.639  38.711   1.00 40.01        O
ATOM    4651   OH2 TIP S 173    -3.162 -13.972   1.056   1.00 37.80        O
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ATOM	4652	OH2	TIP	S	174	15.866	36.292	44.854	1.00 41.03	O
ATOM	4653	OH2	TIP	S	175	28.716	14.934	29.871	1.00 40.86	O
ATOM	4654	OH2	TIP	S	176	12.877	7.462	40.598	1.00 50.68	O
ATOM	4655	OH2	TIP	S	177	6.133	20.704	-4.054	1.00 39.16	O
ATOM	4656	OH2	TIP	S	178	39.969	28.942	25.391	1.00 38.15	O
ATOM	4657	OH2	TIP	S	179	-13.449	0.920	-7.668	1.00 44.30	O
ATOM	4658	OH2	TIP	S	180	-1.907	-19.850	-13.019	1.00 46.61	O
ATOM	4659	OH2	TIP	S	181	-11.803	7.776	20.873	1.00 44.08	O
ATOM	4660	OH2	TIP	S	182	15.943	16.779	25.867	1.00 50.71	O
ATOM	4661	OH2	TIP	S	183	11.887	41.459	29.150	1.00 40.31	O
ATOM	4662	OH2	TIP	S	184	-12.916	-6.604	20.001	1.00 48.89	O
ATOM	4663	OH2	TIP	S	185	37.386	36.717	10.040	1.00 47.31	O
ATOM	4664	OH2	TIP	S	186	2.834	18.279	41.221	1.00 54.64	O
ATOM	4665	OH2	TIP	S	187	-9.066	-0.690	19.812	1.00 43.53	O
ATOM	4666	OH2	TIP	S	188	16.454	33.980	25.756	1.00 38.52	O
ATOM	4667	OH2	TIP	S	189	23.851	22.769	22.843	1.00 48.45	O
ATOM	4668	OH2	TIP	S	190	-14.255	-12.614	8.773	1.00 46.74	O
ATOM	4669	OH2	TIP	S	191	-5.249	-12.948	-12.695	1.00 53.90	O
ATOM	4670	OH2	TIP	S	192	9.039	-20.611	1.774	1.00 42.77	O
ATOM	4671	OH2	TIP	S	193	-5.304	-5.892	-10.918	1.00 47.95	O
ATOM	4672	OH2	TIP	S	194	9.516	-11.723	5.016	1.00 49.40	O
ATOM	4673	OH2	TIP	S	195	20.372	36.265	6.690	1.00 42.55	O
ATOM	4674	OH2	TIP	S	196	9.099	5.271	5.043	1.00 40.29	O
ATOM	4675	OH2	TIP	S	197	28.290	20.438	9.887	1.00 44.18	O
ATOM	4676	OH2	TIP	S	198	41.403	24.242	26.360	1.00 41.99	O
ATOM	4677	OH2	TIP	S	199	17.555	-7.280	-3.972	1.00 45.72	O
ATOM	4678	OH2	TIP	S	200	11.643	26.387	33.558	1.00 44.67	O
ATOM	4679	OH2	TIP	S	201	-13.080	-2.043	17.068	1.00 48.89	O
ATOM	4680	OH2	TIP	S	202	21.406	41.180	6.510	1.00 47.83	O
ATOM	4681	OH2	TIP	S	203	-3.647	-14.349	4.372	1.00 45.03	O
ATOM	4682	OH2	TIP	S	204	1.975	-16.444	0.528	1.00 46.05	O
ATOM	4683	OH2	TIP	S	205	29.352	38.318	42.802	1.00 39.18	O
ATOM	4684	OH2	TIP	S	206	23.761	43.491	42.218	1.00 52.21	O
ATOM	4685	OH2	TIP	S	207	37.832	29.664	12.655	1.00 40.31	O
ATOM	4686	OH2	TIP	S	208	4.964	17.602	2.226	1.00 49.67	O
ATOM	4687	OH2	TIP	S	209	39.168	40.024	22.519	1.00 48.01	O
ATOM	4688	OH2	TIP	S	210	13.868	-18.464	-3.462	1.00 45.96	O
ATOM	4689	OH2	TIP	S	211	-15.848	-4.527	4.594	1.00 44.75	O
ATOM	4690	OH2	TIP	S	212	-10.372	16.898	-0.055	1.00 41.74	O
ATOM	4691	OH2	TIP	S	213	-3.769	9.428	-11.859	1.00 41.64	O
ATOM	4692	OH2	TIP	S	214	-12.248	16.128	8.702	1.00 42.97	O
ATOM	4693	OH2	TIP	S	215	-10.705	-1.226	-13.945	1.00 46.83	O
ATOM	4694	OH2	TIP	S	216	22.402	4.106	44.758	1.00 42.90	O
ATOM	4695	OH2	TIP	S	217	-17.355	1.265	1.310	1.00 49.40	O
ATOM	4696	OH2	TIP	S	218	42.477	37.616	23.340	1.00 42.07	O
ATOM	4697	OH2	TIP	S	219	-16.918	8.816	7.795	1.00 46.92	O
ATOM	4698	OH2	TIP	S	220	27.500	8.859	43.884	1.00 48.46	O
ATOM	4699	OH2	TIP	S	221	30.021	39.029	40.447	1.00 44.55	O
ATOM	4700	OH2	TIP	S	222	39.391	18.850	37.190	1.00 52.09	O
ATOM	4701	OH2	TIP	S	223	4.533	-18.856	1.922	1.00 50.69	O
ATOM	4702	OH2	TIP	S	224	29.183	14.389	26.673	1.00 47.97	O
ATOM	4703	OH2	TIP	S	225	-18.903	-8.822	10.919	1.00 49.49	O
ATOM	4704	OH2	TIP	S	226	29.080	14.271	21.460	1.00 41.94	O
ATOM	4705	OH2	TIP	S	227	-12.418	15.936	-7.420	1.00 49.12	O
ATOM	4706	OH2	TIP	S	228	40.908	38.798	10.820	1.00 48.24	O
ATOM	4707	OH2	TIP	S	229	20.873	22.585	47.103	1.00 50.53	O
ATOM	4708	OH2	TIP	S	230	21.831	-10.033	-6.237	1.00 53.05	O
ATOM	4709	OH2	TIP	S	231	29.823	5.586	31.413	1.00 52.07	O
ATOM	4710	OH2	TIP	S	232	44.472	19.890	19.952	1.00 49.75	O
ATOM	4711	OH2	TIP	S	233	-14.590	-13.479	12.084	1.00 44.70	O
ATOM	4712	OH2	TIP	S	234	36.315	29.168	8.598	1.00 49.27	O
ATOM	4713	OH2	TIP	S	235	-3.492	-14.586	9.423	1.00 44.24	O
ATOM	4714	OH2	TIP	S	236	37.931	44.730	38.212	1.00 52.70	O
ATOM	4715	OH2	TIP	S	237	-13.540	11.244	8.565	1.00 48.15	O
ATOM	4716	OH2	TIP	S	238	-15.408	10.000	20.145	1.00 50.07	O
ATOM	4717	OH2	TIP	S	239	20.743	2.608	48.382	1.00 49.86	O
ATOM	4718	OH2	TIP	S	240	23.597	12.310	30.357	1.00 48.72	O
ATOM	4719	OH2	TIP	S	241	-5.755	-8.661	-12.899	1.00 51.10	O

```
                              atomic coordinates.txt
ATOM   4720  OH2 TIP S 242      40.644  44.705  34.483  1.00 51.24        O
ATOM   4721  OH2 TIP S 243      32.880  11.239  31.811  1.00 48.34        O
ATOM   4722  OH2 TIP S 244      -7.454 -17.415  -0.915  1.00 45.03        O
ATOM   4723  OH2 TIP S 245      13.922  -2.398  -2.504  1.00 46.83        O
ATOM   4724  OH2 TIP S 246       0.782  12.427 -14.770  1.00 48.57        O
ATOM   4725  OH2 TIP S 247     -15.049  15.812  -3.622  1.00 51.01        O
ATOM   4726  OH2 TIP S 248       4.404  15.313  18.746  1.00 47.05        O
ATOM   4727  OH2 TIP S 249      31.402  20.217  43.758  1.00 52.57        O
ATOM   4728  OH2 TIP S 250     -10.062   2.073  -9.809  1.00 50.33        O
ATOM   4729  OH2 TIP S 251      11.650  -0.830   4.614  1.00 50.82        O
ATOM   4730  OH2 TIP S 252      -1.232 -15.435   4.563  1.00 50.12        O
ATOM   4731  OH2 TIP S 253     -12.330   0.786  18.255  1.00 43.46        O
ATOM   4732  OH2 TIP S 254      36.403  27.682  44.769  1.00 51.60        O
ATOM   4733  OH2 TIP S 255     -18.273   6.055   3.212  1.00 51.88        O
ATOM   4734  OH2 TIP S 256     -13.609  16.893  -0.632  1.00 50.05        O
ATOM   4735  OH2 TIP S 257      14.001  15.235   0.255  1.00 48.29        O
ATOM   4736  OH2 TIP S 258      10.461   2.911   6.999  1.00 51.70        O
ATOM   4737  OH2 TIP S 259      11.740  10.308  34.387  1.00 49.96        O
ATOM   4738  OH2 TIP S 260     -11.901   5.018  -8.016  1.00 50.95        O
ATOM   4739  OH2 TIP S 261     -10.492  19.957  -5.817  1.00 45.58        O
TER       1      TIP S 261
END
```

Table 2: Crystal Data and X-ray data statistics

Number of crystals	1
Space group	P1 (primitive triclinic)
Unit cell dimensions	a = 35.77 b = 57.56 c = 80.20Å
	α = 68.97 β = 89.83 γ = 89.95°
Number of monomers / a.u.	2
Packing coefficient	2.05Å³/Da
Solvent content	38%
Resolution range	50 – 1.9Å
Number of observations	386926
Number of reject observations	24465
Number of unique reflections	46855
Mosaicity	0.817
Overall	
Data redundancy	8.25
Data completeness	97.0%
< I/ σ (I)>	20.6
R_{merge}	0.049
Highest resolution shell	
Resolution range	1.97-1.90Å
Completeness for shell	96.5%
R_{merge} for shell	0.175
Reflections with I ≥ 3σ(I)	86.7%

Table 3: Refinement Statistics

Data used in refinement	
- resolution range	19.26-1.90Å
- intensity cutoff (Sigma(F))	0.0
- number of reflections	45463
- completeness (working +test set)	96.7%
-test set	5.0%
Fit to data used in refinement	
- overall R_{cryst}	0.182
- overall R_{free}	0.209
Fit in the highest resolution bin	
- resolution range	2.02 - 1.90 Å
- bin completeness (working +test set)	93.7%
- bin R_{cryst}	0.195
- bin R_{free}	0.241
Number of non-hydrogen atoms	
- protein atoms	4478
- ligand (2 molecules staurosporin)	70
- waters	261

Overall B value from Wilson plot	24.1Å²
Overall mean B value	35.0Å²
Cross-validated estimated coordinate error (low res. cutoff: 5.0Å)	
- from Luzzati plot	0.22Å
- from σ_A	0.11Å
Rms deviations from ideal values	0.011Å
- bond lengths	1.3°
- bond angles	21.4°
- dihedral angles	0.91°
- improper angles	

Table 4: List of Contacts Between Catalytic Domain of ZAP-70 and Staurosporine

```
atom in protein      atom in staurosporine     distance (A)
================================================================

    LEU 344 O         STU  C25        3.4
    GLY 345 CA        STU  O4         3.5
    CYS 346 O         STU  C26        3.9
    GLY 347 N         STU  C26        5.4
    PHE 349 CZ        STU  C16        4.5
    VAL 352 CG2       STU  C17        3.8
    ALA 367 CB        STU  N1         3.2
    LYS 369 CD        STU  C14        4.3
    GLU 386 OE2       STU  C14        4.4
    VAL 399 CG1       STU  C9         4.1
    MET 414 CE        STU  C13        3.6
    GLU 415 O         STU  N1         3.0    H-bridge
    MET 416 CA        STU  O5         3.4
    ALA 417 N         STU  O5         2.7    H-bridge
    GLY 418 O         STU  C3         4.3
    GLY 419 C         STU  C3         4.8
    GLY 420 CA        STU  C3         3.5
    PRO 421 CG        STU  C24        3.8
    HIS 423 NE2       STU  N4         5.1        through Solv3
    Lys 424 NZ        STU  N4         6.4    through Solv3
    ARG 465 O         STU  N4         3.0        H-bridge
    ASN 466 OD1       STU  C27        3.4
    LEU 468 CD1       STU  C7         3.3
    SER 478 OG        STU  C27        3.1        Alt. Pos.
    ASP 479 CG        STU  C15        3.5
```